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Holomorphy of the Scattering Matrix with Respect to c^{-2} for Dirac Operators and an Explicit Treatment of Relativistic Corrections

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Abstract. We prove holomorphy of the scattering matrix at fixed energy with respect to c^{-2} for abstract Dirac operators. Relativistic corrections of order c^{-2} to the nonrelativistic limit scattering matrix (associated with an abstract Pauli Hamiltonian) are explicitly determined. As applications of our abstract approach we discuss concrete realizations of the Dirac operator in one and three dimensions and explicitly compute relativistic corrections of order c^{-2} of the reflection and transmission coefficients in one dimension and of the scattering matrix in three dimensions. Moreover, we give a comparison between our approach and the first-order relativistic corrections according to Foldy-Wouthuysen scattering theory and show complete agreement of the two methods.

1. Introduction

We provide a general framework for the nonrelativistic limit of scattering theory for general Dirac operators. Our treatment is based on an abstract approach employed in [10, 11] to obtain explicit expressions for first order corrections of bound state energies with respect to c^{-2}.

Historically, the first rigorous treatment of the nonrelativistic limit of Dirac Hamiltonians seems to go back Titchmarsh [36] who proved holomorphy of the Dirac eigenvalues (rest energy subtracted) with respect to c^{-2} for spherically symmetric potentials and obtained explicit formulas for relativistic bound state corrections of order $O(c^{-2})$ (formally derived in [32]). Holomorphy of the Dirac resolvent in three dimensions in c^{-1} for electrostatic interactions were first obtained by Veselic [38] and then extended to electromagnetic interactions by Hunziker [16]. An entirely different approach, based on an abstract set up, has been used in [6] to prove strong convergence of the unitary groups as $c^{-1} \to \infty$. Employing this abstract framework, holomorphy of the Dirac resolvent in c^{-1} under general conditions on the electromagnetic interaction potentials has been obtained in [10, 11]. Moreover, this approach led to the first rigorous derivation of explicit formulas for relativistic corrections of order $O(c^{-2})$ to bound state energies. (Earlier, a justification of the fact that formal perturbation theory according to Foldy and Wouthuysen yields correct results has been given in terms of spectral concentration in [12, 37].) In the case of eigenvalue degeneracies of the unperturbed Pauli Hamiltonian, an extension of the results in [10, 11] appeared in [41] (see also [14]). Relativistic corrections for energy bands and corresponding corrections for impurity bound states for one-dimensional periodic systems were treated in [5]. Convergence of solutions of the Dirac equation based on semi-group methods have also been obtained in [31].

Much less activity has been devoted to the nonrelativistic limit of the Dirac scattering theory. In fact, we are only aware of the proof of strong convergence of wave and scattering operators as $c^{-1} \to \infty$ in [39] and [42] and a recent treatment of the scattering amplitude in [14] based on a different approach.

In Sect. 2, based on the abstract approach of [6], we summarize the main results of [10, 11] concerning the holomorphy of the Dirac resolvent operator with respect to c^{-2} near $c^{-2} = 0$. In Sect. 3 we review some of the results of [22] on abstract scattering theory needed in Sects. 4 and 5. Our main result on the holomorphic expansion of the abstract scattering matrix in c^{-2} around its nonrelativistic counterpart at $c^{-2} = 0$ is established in Sect. 4. We also provide an explicit formula for the correction term of order c^{-2} of the scattering matrix in terms of nonrelativistic scattering quantities (see Theorem 4.2). Concrete realizations of our abstract approach in Sect. 4 in one and three dimensions are presented in Sect. 5. In particular, we explicitly compute relativistic corrections of order c^{-2} of the reflection and transmission coefficients in one dimension and of the scattering matrix in three dimensions. Finally we compare our approach and the first order relativistic corrections according to Foldy-Wouthuysen scattering theory and show complete agreement of the two methods in Appendix A.

2. The Abstract Approach

The aim of this section is to summarize the main results obtained in [10, 11] (based on the abstract approach of [6]) concerning holomorphy of the Dirac resolvent operator with respect to c^{-2} near $c^{-2} = 0$. Let $\mathscr{H}_j$, $j = 1, 2$ be separable, complex Hilbert spaces and introduce self-adjoint operators α, β in $\mathscr{H} = \mathscr{H}_1 \oplus \mathscr{H}_2$ of the type

$$\alpha = \begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.1}$$

where A is a densely defined, closed operator from $\mathscr{H}_1$ into $\mathscr{H}_2$. Next, we introduce the abstract free Dirac operator $H^0(c)$ by

$$H^0(c) = c\alpha + mc^2\beta, \quad \mathscr{D}(H^0(c)) = \mathscr{D}(\alpha), \quad c \in \mathbb{R}\backslash\{0\}, \quad m > 0 \tag{2.2}$$

and the interaction V by

$$V = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}, \tag{2.3}$$

where V_j denotes self-adjoint operators in $\mathscr{H}_j$, $j = 1, 2$, respectively. Assuming V_1 (respectively V_2) to be bounded with respect to A (respectively A^*), i.e.,

$$\mathscr{D}(A) \subseteq \mathscr{D}(V_1), \quad \mathscr{D}(A^*) \subseteq \mathscr{D}(V_2), \tag{2.4}$$

the abstract Dirac operator $H(c)$ reads

$$H(c) = H^0(c) + V, \quad \mathscr{D}(H(c)) = \mathscr{D}(\alpha). \tag{2.5}$$

Obviously $H(c)$ is self-adjoint for $|c|$ large enough. The corresponding self-adjoint (free) Pauli operators in $\mathscr{H}_j$, $j = 1,2$ are then defind by

$$H_1^0 = (2m)^{-1}A^*A, \qquad H_2^0 = (2m)^{-1}AA^*, \tag{2.6}$$

$$H_1 = H_1^0 + V_1, \qquad \mathscr{D}(H_1) = \mathscr{D}(A^*A), \tag{2.7}$$

$$H_2 = H_2^0 + V_2, \qquad \mathscr{D}(H_2) = \mathscr{D}(AA^*). \tag{2.8}$$

Introducing in $\mathscr{H}$ the operator $B(c)$ [16]

$$B(c) = \begin{pmatrix} 1 & 0 \\ 0 & c \end{pmatrix}, \tag{2.9}$$

we recall [10, 11].

Theorem 2.1. *Let $H(c)$ be defined as above and fix $z \in \mathbb{C}\backslash\mathbb{R}$. Then*
(i) *$(H(c) - mc^2 - z)^{-1}$ is holomorphic with respect to c^{-1} around $c^{-1} = 0$,*

$$\begin{aligned}&(H(c) - mc^2 - z)^{-1}\\ &= \left\{1 + \begin{pmatrix} 0 & (2mc)^{-1}(H_1 - z)^{-1}A^*(V_2 - z) \\ (2mc)^{-1}A(H_1^0 - z)^{-1}V_1 & (2mc^2)^{-1}z(H_2^0 - z)^{-1}(V_2 - z) \end{pmatrix}\right\}^{-1}\\ &\quad\times \begin{pmatrix} (H_1 - z)^{-1} & (2mc)^{-1}(H_1 - z)^{-1}A^* \\ (2mc)^{-1}A(H_1^0 - z)^{-1} & (2mc^2)^{-1}z(H_2^0 - z)^{-1} \end{pmatrix}.\end{aligned} \tag{2.10}$$

(ii) *$B(c)\,(H(c) - mc^2 - z)^{-1}B(c)^{-1}$ is holomorphic with respect to c^{-2} around $c^{-2} = 0$,*

$$\begin{aligned}&B(c)\,(H(c) - mc^2 - z)^{-1}B(c)^{-1}\\ &= \left\{1 + \begin{pmatrix} 0 & (2mc^2)^{-1}(H_1 - z)^{-1}A^*(V_2 - z) \\ 0 & (2mc^2)^{-1}[(2m)^{-1}A(H_1 - z)^{-1}A^* - 1]\,(V_2 - z) \end{pmatrix}\right\}^{-1}\\ &\quad\times \begin{pmatrix} (H_1 - z)^{-1} & (2mc^2)^{-1}(H_1 - z)^{-1}A^* \\ (2m)^{-1}A(H_1 - z)^{-1} & (2mc^2)^{-1}[(2m)^{-1}A(H_1 - z)^{-1}A^* - 1] \end{pmatrix}.\end{aligned} \tag{2.11}$$

First order expansions in (2.10) and (2.11) yield

$$\begin{aligned}&(H(c) - mc^2 - z)^{-1}\\ &= \begin{pmatrix} (H_1 - z)^{-1} & 0 \\ 0 & 0 \end{pmatrix}\\ &\quad + c^{-1}\begin{pmatrix} 0 & (2m)^{-1}(H_1 - z)^{-1}A^* \\ (2m)^{-1}A(H_1 - z)^{-1} & 0 \end{pmatrix} + O(c^{-2})\end{aligned} \tag{2.12}$$

(clearly illustrating the nonrelativistic limit $|c| \to \infty$) and

$$\begin{aligned}&B(c)\,(H(c) - mc^2 - z)^{-1}B(c)^{-1}\\ &= \begin{pmatrix} (H_1 - z)^{-1} & 0 \\ (2m)^{-1}A(H_1 - z)^{-1} & 0 \end{pmatrix} + c^{-2}\begin{pmatrix} R_{11}(z) & R_{12}(z) \\ R_{21}(z) & R_{22}(z) \end{pmatrix} + O(c^{-4})\\ &:= R^{(0)}(z) + c^{-2}R^{(1)}(z) + O(c^{-4}),\end{aligned} \tag{2.13}$$

$$\begin{aligned}&R_{11}(z) = (2m)^{-2}(H_1 - z)^{-1}A^*(z - V_2)A(H_1 - z)^{-1},\\ &R_{12}(z) = (2m)^{-1}(H_1 - z)^{-1}A^*,\\ &R_{21}(z) = (2m)^{-2}[(2m)^{-1}A(H_1 - z)^{-1}A^* - 1]\,(z - V_2)A(H_1 - z)^{-1},\\ &R_{22}(z) = (2m)^{-1}[(2m)^{-1}A(H_1 - z)^{-1}A^* - 1].\end{aligned} \tag{2.14}$$

3. On Abstract Scattering Theory

In this section we summarize some of the results on abstract scattering theory obtained by Kuroda [22] which are most relevant to us in Sects. 4 and 5. For additional material on scattering theory in the present context we refer to [1–4, 7, 17, 19, 23–25, 28].

We define in the Hilbert space $\mathscr{H} = \mathscr{H}_1 \oplus \mathscr{H}_2$,

$$\hat{H}_1 := H^0(c) - mc^2, \qquad \hat{H}_2 := H(c) - mc^2 \tag{3.1}$$

and introduce the following factorisation of V:

$$V_j = v_j^{1/2} |v_j|^{1/2}, \qquad j = 1, 2, \tag{3.2}$$

where

$$v_j^{1/2} := U_j |V_j|^{1/2}, \qquad |v_j|^{1/2} := |V_j|^{1/2}, \qquad j = 1, 2 \tag{3.3}$$

with $V_j = U_j |V_j|$ the polar decomposition of V_j,

$$Y := B(c)^{-1} \begin{pmatrix} |v_1|^{1/2} & 0 \\ 0 & |v_2|^{1/2} \end{pmatrix} = \begin{pmatrix} |v_1|^{1/2} & 0 \\ 0 & \frac{1}{c} |v_2|^{1/2} \end{pmatrix}, \tag{3.4}$$

$$Z := B(c) \begin{pmatrix} v_1^{1/2} & 0 \\ 0 & v_2^{1/2} \end{pmatrix} = \begin{pmatrix} v_1^{1/2} & 0 \\ 0 & c v_2^{1/2} \end{pmatrix}, \tag{3.5}$$

$$R_j(z) := (\hat{H}_j - z)^{-1}, \qquad z \in \varrho(\hat{H}_j), \qquad j = 1, 2. \tag{3.6}$$

The following assumptions 3.1–3.3 and 3.5–3.8 are basic in the approach of [22]:

Assumption 3.1. Y and Z are closed operators from $\mathscr{H}$ to another Hilbert space $\mathscr{K} = \mathscr{K}_1 \oplus \mathscr{K}_2$ with $\mathscr{D}(\hat{H}_1) \subseteq \mathscr{D}(Y)$ and $\mathscr{D}(\hat{H}_1) \subseteq \mathscr{D}(Z)$.
(This implies that $Y R_1(z)$, $Z R_1(z) \in \mathscr{B}(\mathscr{H}, \mathscr{K})$, see [18, p. 191].)

Assumption 3.2. $Z R_1(z) Y^*$ is closable and the closure of $Z R_1(z) Y^* \in \mathscr{B}(\mathscr{K})$ for one (or equivalently for all) $z \in \varrho(\hat{H}_1)$,

$$Q_1(z, c) := [Z R_1(z) Y^*]^{(a)}, \qquad G_1(z, c) := 1 + Q_1(z, c), \tag{3.7}$$

where $^{(a)}$ denotes the closure.

Assumption 3.3. Let $z \in \varrho(\hat{H}_1) \cap \varrho(\hat{H}_2)$. Then $G_1(z, c)^{-1} \in \mathscr{B}(\mathscr{K})$ and

$$R_2(z) = R_1(z) - [R_1(z) Y^*]^a G_1(z)^{-1} Z R_1(z). \tag{3.8}$$

Thus Propositions 2.6 and 2.7 in [22] hold: Define

$$Q_2(z, c) := [Z R_2(z) Y^*]^{(a)}, \qquad G_2(z, c) := 1 - Q_2(z, c), \qquad z \in \varrho(\hat{H}_2). \tag{3.9}$$

Then

$$G_2(z, c) = G_1(z, c)^{-1}, \qquad z \in \varrho(\hat{H}_2). \tag{3.10}$$

Remark 3.4. From our assumptions on $H^0(c)$ and V in Chapter 2 we infer that

(i) $V^{1/2}$ is $\hat{H}^0(c)$ bounded with bound 0 and hence Assumption 3.1 is fulfilled.
(ii) $V^{1/2}$ is $\hat{H}^0(c)^{1/2}$ bounded implying that Assumption 3.2 is fulfilled.
(iii) The second resolvent equation gives

$$\begin{aligned} (1 + [Z R_1(z) Y^*]^{(a)}) (1 - [Z R_2(z) Y^*]^{(a)}) &= 1, \\ (1 - [Z R_2(z) Y^*]^{(a)}) (1 + [Z R_1(z) Y^*]^{(a)}) &= 1 \end{aligned} \tag{3.11}$$

(see e.g. [1, p. 369]) and thus Assumption 3.3 is fulfilled.

Next let E_j denote the spectral measures associated with $\hat{H}_j$, $j = 1, 2$.

Assumption 3.5. There exists a Hilbert space $\mathscr{C}$, a non-empty open set $I \subseteq \mathbb{R}$, and a unitary operator F from $E_1(I)\mathscr{H}$ onto $L^2(I;\mathscr{C})$ such that for every Borel set $I' \subseteq I$ one has $FE_1(I')F^{-1} = \chi_{I'}$, where $\chi_{I'}$ denotes the operator of multiplication by the characteristic function of I'.

Assumption 3.6. There exist $B(\mathscr{K},\mathscr{C})$-valued functions $T(\lambda,c,Y)$ and $T(\lambda,c,Z)$, $\lambda \in I$, such that
(i) $T(\cdot,c,Y)$ and $T(\cdot,c,Z)$ are locally Hölder continuous in I with respect to the operator norm.
(ii) There exist dense subsets $D \subseteq \mathscr{D}(Y^*)$ and $D' \subseteq \mathscr{D}(Z^*)$ such that for any $u \in D$ and $v \in D'$ one has

$$\begin{aligned} T(\lambda,c,Y)u &= (FE_1(I)Y^*u)(\lambda), \\ T(\lambda,c,Z)v &= (FE_1(I)Z^*v)(\lambda), \end{aligned} \quad \text{for a.e. } \lambda \in I. \tag{3.12}$$

Assumption 3.7. For one (or equivalently all) $z \in \varrho(\hat{H}_1)$ either

$$YR_1(z) \in B_\infty(\mathscr{H},\mathscr{K}) \quad \text{or} \quad ZR_1(z) \in B_\infty(\mathscr{H},\mathscr{K}).$$

Here $B_\infty(\mathscr{H},\mathscr{K})$ denotes the set of compact operators from $\mathscr{H}$ to $\mathscr{K}$.

Assumption 3.8. The subspace generated by $\{E_j(I')Y^*u \mid u \in \mathscr{D}(Y^*),\ I' \subseteq I \text{ a Borel set}\}$ is dense in $E_j(I)\mathscr{H}$, $j = 1, 2$.

Remark 3.9 [22]. Since $\mathscr{H}$ is separable, Assumption 3.5 is equivalent to assuming that $\hat{H}_1$ has absolutely continuous spectrum in I with constant multiplicity. Moreover, $\mathscr{C}$ is determined uniquely up to unitary equivalence and F is uniquely determined up to unitary equivalence with decomposable, unitary operators on $L^2(I;\mathscr{C})$.

Since these assumptions are identical with the ones in [22] we have all the results of [22, Sect. 3 and 4] at our disposal; e.g., the norm limits

$$G_{1\pm}(\lambda,c) := n - \lim_{\varepsilon\downarrow 0} G_1(\lambda \pm i\varepsilon, c), \qquad Q_{1\pm}(\lambda,c) := n - \lim_{\varepsilon\downarrow 0} Q_1(\lambda \pm i\varepsilon, c) \tag{3.13}$$

exist (see [22, Theorem 3.9]) and introducing

$$e_\pm(c) := \{\lambda \in I \mid G_{1\pm}(\lambda,c) \text{ is not one to one}\}, \qquad e(c) := e_+(c) \cup e_-(c) \tag{3.14}$$

($e(c)$ is a closed set of Lebesgue measure zero [22]) we get for $\lambda \in I\backslash e_\pm(c)$ the existence of the boundary values

$$G_{2\pm}(\lambda,c) = n - \lim_{\varepsilon\downarrow 0} G_2(\lambda \pm i\varepsilon, c) \tag{3.15}$$

and

$$G_{2\pm}(\lambda,c) = G_{1\pm}(\lambda,c)^{-1} \tag{3.16}$$

(see [22, Theorem 3.10]).

Also Theorems 3.11–3.13 and 6.3 of [22] are valid. In particular, we obtain for the fibers of the scattering operator

Theorem 3.10 [22]. *For $\lambda \in I\backslash e(c)$ the scattering matrix $S(\lambda,c)$ in $\mathscr{C}$ associated with the pair $(\hat{H}_2, \hat{H}_1)$ is given by*

$$S(\lambda,c) = 1 - 2\pi i T(\lambda,c,Y)G_{2+}(\lambda,c)T(\lambda,c,Z)^*. \tag{3.17}$$

$S(\cdot,c)$ is unitary in $\mathscr{C}$ and locally Hölder continuous on $I\backslash e(c)$ with respect to the norm in $\mathscr{B}(\mathscr{C})$.

4. Holomorphy of the Scattering Matrix in c^{-2} and Relativistic Corrections

In this section we combine Sects. 2 and 3 and establish a holomorphic expansion of the abstract scattering matrix with respect to c^{-2} around its nonrelativistic counterpart at $c^{-2} = 0$. Moreover, we explicitly determine the first correction of the scattering matrix of order c^{-2} in terms of nonrelativistic scattering quantities in Theorem 4.2.

Let $I \subseteq \mathbb{R}^+ := (0, \infty)$ and define

$$I_{\pm 0} := \{\lambda \mid \lambda \in I \backslash e_\pm(c^{-2} = 0)\}, \qquad I_0 = I_{+0} \cap I_{-0}. \tag{4.1}$$

In addition we strengthen Assumptions 3.2 and 3.6 by introducing

Assumption 4.1. (i) For $\lambda \in I$, $T(\lambda, c, Y)$ and $T(\lambda, c, Z)$ are holomorphic in c^{-2} around $c^{-2} = 0$ and

(ii) for $\lambda \in I_{+0}$

$$Q_{1+}(\lambda, c) = \lim_{\varepsilon \downarrow 0} Q_{1+}(\lambda + i\varepsilon, c) \tag{4.2}$$

is holomorphic in c^{-2} around $c^{-2} = 0$.

Based on Theorem 2.1 we now turn to the expansion of $G_{2+}(\lambda, c)$, $\lambda \in I_{+0}$,

$$\begin{aligned} G_{2+}(\lambda, c) &= (G_{1+}(\lambda, c))^{-1} = (1 + Q_{1+}(\lambda, c))^{-1} = \lim_{\varepsilon \downarrow 0} (1 + Z R_1(\lambda + i\varepsilon) Y^*)^{-1} \\ &= \lim_{\varepsilon \downarrow 0} \left\{ 1 + Z \left(\begin{pmatrix} 0 & cA^* \\ cA & -2mc^2 \end{pmatrix} - (\lambda + i\varepsilon) \right)^{-1} Y^* \right\}^{-1} \\ &:= G_{2+}^{(0)}(\lambda) + \frac{1}{c^2} G_{2+}^{(1)}(\lambda) + O(c^{-4}), \end{aligned} \tag{4.3}$$

where $^{(n)}$, $n \in \mathbb{N}_0$ denotes the order of the expansion involved. [Since $G_{2+}(\lambda, c) = \lim_{\varepsilon \downarrow 0} G_2(\lambda + i\varepsilon, c)$ is continuous in $z = \lambda + i\varepsilon$, and holomorphic in c^{-2} we may interchange the limits.]

Next define

$$\begin{aligned} g_2(z) &:= (1 + v_1^{1/2}(H_1^0 - z)^{-1}|v_1|^{1/2})^{-1}, \qquad z = \lambda + i\varepsilon, \varepsilon > 0, \\ g_{2\pm}(\lambda) &:= \lim_{\varepsilon \downarrow 0} g_2(\lambda \pm i\varepsilon). \end{aligned} \tag{4.4}$$

We then get

$$G_{2+}^{(0)}(\lambda) = \lim_{\varepsilon \downarrow 0} \begin{pmatrix} g_2(z) & 0 \\ -v_2^{1/2} \dfrac{A}{2m} (H_1^0 - z)^{-1}|v_1|^{1/2} g_2(z) & 1 \end{pmatrix}, \qquad z = \lambda + i\varepsilon \tag{4.5}$$

and

$$G_{2+}^{(1)}(\lambda) = \lim_{\varepsilon \downarrow 0} \begin{pmatrix} b_{11}(z) & b_{12}(z) \\ b_{21}(z) & b_{22}(z) \end{pmatrix}, \qquad z = \lambda + i\varepsilon, \tag{4.6}$$

with

$$\begin{aligned}
b_{11}(z) &= -g_2(z)v_1^{1/2}R_{11}(z)|v_1|^{1/2}g_2(z) \\
&\quad + g_2(z)v_1^{1/2}R_{12}(z)|v_2|^{1/2}v_2^{1/2}\frac{A}{2m}(H_1^0-z)^{-1}|v_1|^{1/2}g_2(z), \\
b_{12}(z) &= -g_2(z)v_1^{1/2}R_{12}(z)|v_2|^{1/2}, \\
b_{21}(z) &= v_2^{1/2}\frac{A}{2m}(H_1^0-z)^{-1}|v_1|^{1/2}g_2(z)v_1^{1/2}R_{11}(z)|v_1|^{1/2}g_2(z) \\
&\quad - v_2^{1/2}R_{21}(z)|v_1|^{1/2}g_2(z) - v_2^{1/2}\frac{A}{2m}(H_1^0-z)^{-1}|v_1|^{1/2}g_2(z) \\
&\quad \times v_1^{1/2}R_{12}(z)|v_2|^{1/2}v_2^{1/2}\frac{A}{2m}(H_1^0-z)^{-1}|v_1|^{1/2}g_2(z) \\
&\quad + v_2^{1/2}R_{22}(z)|v_2|^{1/2}v_2^{1/2}\frac{A}{2m}(H_1^0-z)^{-1}|v_1|^{1/2}g_2(z), \\
b_{22}(z) &= v_2^{1/2}\frac{A}{2m}(H_1^0-z)^{-1}|v_1|^{1/2}g_2(z)v_1^{1/2}R_{12}(z)|v_2|^{1/2} \\
&\quad - v_2^{1/2}R_{22}(z)|v_2|^{1/2},
\end{aligned} \tag{4.7}$$

where (cf. 2.14)

$$\begin{aligned}
R_{11}(z) &= (2m)^{-2}z(H_1^0-z)^{-1}A^*A(H_1^0-z)^{-1}, \\
R_{12}(z) &= (2m)^{-1}(H_1^0-z)^{-1}A^*, \\
R_{21}(z) &= (2m)^{-2}z^2(H_1^0-z)^{-1}A(H_1^0-z)^{-1}, \\
R_{22}(z) &= (2m)^{-1}z(H_1^0-z)^{-1}.
\end{aligned} \tag{4.8}$$

Next we turn to the operators $T(\lambda, c, Y)$ and $T(\lambda, c, Z)^*$, $\lambda \in I$. We introduce the abbreviations

$$k^d(\lambda, c) := \sqrt{2m\lambda\left(1+\frac{\lambda}{2mc^2}\right)}, \qquad k_0(\lambda, c) := \frac{ck^d(\lambda, c)}{\lambda + 2mc^2}, \qquad \lambda > 0. \tag{4.9}$$

If $\lambda \in (\lambda_1, \lambda_2) = I$, then $k^d(\lambda, c) \in \left(\sqrt{2m\lambda_1}\sqrt{1+\frac{\lambda_1}{2mc^2}}, \sqrt{2m\lambda_2}\sqrt{1+\frac{\lambda_2}{2mc^2}}\right) =: \tilde{I}$.

(Especially in the case $I = (0, \infty)$ we have $I = \tilde{I} = \tilde{I}^2 = (0, \infty)$.)

By Assumption 3.5, α^2 and hence A^*A, AA^* are absolutely continuous in $\tilde{I}^2$ with constant multiplicity.

Now we consider the analogs U_0, M of F and T when A^*A replaces $\hat{H}_1$. Let U_0 be the unitary operator that diagonalizes A^*A on $\tilde{I}^2$. For $h \in E_0(\tilde{I}^2)\mathscr{H}_1$ (where $E_0(\cdot)$ denotes the spectral measure for A^*A) U_0 yields

$$U_0 : E_0(\tilde{I}^2)\mathscr{H}_1 \to L^2(\tilde{I}^2, d\mu; \mathscr{C}), \qquad (U_0A^*Ah)(\mu) = \mu(U_0h)(\mu), \qquad \mu \in \tilde{I}^2. \tag{4.10}$$

In addition we need the operator $M(k, D) : \mathscr{D}(D) \to \mathscr{C}$, where $D : \mathscr{D}(D) \to \mathscr{H}_1$, $\mathscr{D}(D) \subseteq \mathscr{K}_1$ or $\mathscr{K}_2$, D closed

$$M(k, D)h = (U_0E_0(\tilde{I}^2)Dh)(k^2), \qquad h \in \mathscr{D}(D), \qquad k := \sqrt{\mu}, \qquad \text{for a.e. } k \in \tilde{I}. \tag{4.11}$$

In concrete applications the closure of $M(k, D)$ will be a Hilbert Schmidt operator. This closure is then denoted by $M(k, D)$, too.

Now we are in position to construct the unitary operator F that diagonalizes $H^0(c) - mc^2$ on $I \subseteq \mathbb{R}^+$. For $f \in E_1(I, c)\mathscr{H}$ (where $E_1(\cdot, c)$ denotes the spectral measure for $H^0(c) - mc^2$) F yields

$$F : E_1(I, c)\mathscr{H} = E_1(I, c)\,(\mathscr{H}_1 \oplus \mathscr{H}_2) \to L^2(I, d\lambda; \mathscr{C}),$$

$$(Ff)\,(\lambda) = \sqrt{\frac{k^d}{ck_0}}\left((U_0 f_1) + \frac{k_0}{k^d}\,(U_0 A^* f_2)\right)((k^d)^2), \qquad f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \tag{4.12}$$

$$(F[H^0(c) - mc^2]f)\,(\lambda) = \lambda(Ff)\,(\lambda), \qquad \lambda \in I \subseteq \mathbb{R}^+. \tag{4.13}$$

We note that on the subspace of positive energies the abstract Foldy-Wouthuysen transformation coincides with the abstract spectral transformation (see [33, 34]). The representation (4.12), (4.13) is due to the supersymmetric structure of α.

Given these facts we can now express $T(\lambda, c, Y) : \mathscr{H} \to \mathscr{C}$, $\lambda \in I$ in terms of M from (4.11) in the form

$$\begin{aligned} T(\lambda, c, Y)f &= \sqrt{\frac{k^d}{ck_0}}\left[M(k^d, |v_1|^{1/2})f_1 + \frac{k_0}{ck^d}\,M(k^d, A^*|v_2|^{1/2})f_2\right], \\ f &= \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \in \mathscr{H}. \end{aligned} \tag{4.14}$$

For $T(\lambda, c, Z)^* : \mathscr{C} \to \mathscr{H}$, $\lambda \in I$, we get

$$T(\lambda, c, Z)^* h = \sqrt{\frac{k^d}{ck_0}}\begin{pmatrix} M(k^d, v_1^{1/2})^* h \\ \frac{ck_0}{k^d}\,M(k^d, A^* v_2^{1/2})^* h \end{pmatrix}, \qquad h \in \mathscr{C}. \tag{4.15}$$

Now we can expand $T(\lambda, c, Y)$ and $T(\lambda, c, Z)^*$, $\lambda \in I$ with respect to c^{-2} as follows: Define

$$k^s := \sqrt{2m\lambda} \tag{4.16}$$

then, for $|c^{-2}|$ small enough,

$$T(\lambda, c, Y) = \sum_{j=0}^{\infty} c^{-2j}\,T^{(j)}(\lambda, Y), \tag{4.17}$$

$$T(\lambda, c, Z)^* = \sum_{j=0}^{\infty} c^{-2j}\,T^{(j)}(\lambda, Z)^*, \tag{4.18}$$

where

$$T^{(0)}(\lambda, Y) = \sqrt{2m}\,(M(k^s, |v_1|^{1/2}) \;\; 0), \tag{4.19}$$

$$T^{(0)}(\lambda, Z)^* = \sqrt{2m}\begin{pmatrix} M(k^s, v_1^{1/2})^* \\ \frac{1}{2m}\,M(k^s, A^* v_2^{1/2})^* \end{pmatrix}, \tag{4.20}$$

$$\begin{aligned} T^{(1)}(\lambda, Y) &= \sqrt{2m}\,\frac{(k^s)^2}{8m^2}\,(M(k^s, |v_1|^{1/2}) \;\; 0) \\ &\quad + \sqrt{2m}\left(\frac{(k^s)^3}{8m^2}\,M'(k^s, |v_1|^{1/2}) \;\; \frac{1}{2m}\,M(k^s, A^*|v_2|^{1/2})\right) \end{aligned} \tag{4.21}$$

where $M'(k^s, |v_1|^{1/2})$ denotes the derivative of $M(k, |v_1|^{1/2})$ with respect to k at $k = k^s$ and

$$T^{(1)}(\lambda, Z)^* = \sqrt{2m}\,\frac{(k^s)^2}{8m^2}\begin{pmatrix} M(k^s, v_1^{1/2})^* \\ \frac{1}{2m} M(k^s, A^* v_2^{1/2})^* \end{pmatrix}$$
$$+ \sqrt{2m}\begin{pmatrix} \frac{(k^s)^3}{8m^2} M'(k^s, v_1^{1/2})^* \\ -\frac{(k^s)^2}{8m^3} M(k^s, A^* v_2^{1/2})^* + \frac{(k^s)^3}{16m^3} M'(k^s, A^* v_2^{1/2})^* \end{pmatrix}. \tag{4.22}$$

We can now state the following result for the fibers of the scattering operator.

Theorem 4.2. *For $\lambda \in I_0$, the scattering matrix $S(\lambda, c)$ associated with the pair $(H(c) - mc^2,\ H^0(c) - mc^2)$ is holomorphic in c^{-2} around $c^{-2} = 0$ and we get the following expansion:*

$$S(\lambda, c) = 1 - 2\pi i T(\lambda, c, Y) G_{2+}(\lambda, c) T(\lambda, c, Z)^* = \sum_{j=0}^{\infty} c^{-2j} S^{(j)}(\lambda)$$
$$= S^0(\lambda) - \frac{1}{c^2}\, 2\pi i \{T^{(1)}(\lambda, Y) G_{2+}^{(0)}(\lambda) T^{(0)}(\lambda, Z)^*$$
$$+ T^{(0)}(\lambda, Y) G_{2+}^{(1)}(\lambda) T^{(0)}(\lambda, Z)^* + T^{(0)}(\lambda, Y) G_{2+}^{(0)}(\lambda) T^{(1)}(\lambda, Z)^*\}$$
$$+ O(c^{-4}). \tag{4.23}$$

We therefore get

$$S^{(0)}(\lambda) = 1 - 2\pi i\{2m M(k^s, |v_1|^{1/2}) g_{2+}(\lambda) M(k^s, v_1^{1/2})^*\}, \qquad \lambda \in I_0, \tag{4.24}$$

the scattering matrix for the associated pair of Pauli operators (H_1, H_1^0) (illustrating the non-relativistic limit) and the explicit correction term of order c^{-2},

$$S^{(1)}(\lambda) = \frac{(k^s)^2}{4m^2}(S^{(0)}(\lambda) - 1) - 2\pi i\Big\{\frac{(k^s)^3}{4m} M'(k^s, |v_1|^{1/2}) g_{2+}(\lambda) M(k^s, v_1^{1/2})^*$$
$$- \frac{1}{2m} M(k^s, A^*|v_2|^{1/2})[v_2^{1/2} A (H_1^0 - \lambda - i0)^{-1} |v_1|^{1/2}] g_{2+}(\lambda) M(k^s, v_1^{1/2})^*$$
$$+ \frac{1}{2m} M(k^s, A^*|v_2|^{1/2}) M(k^s, A^* v_2^{1/2})^*$$
$$+ \frac{(k^s)^3}{4m} M(k^s, |v_1|^{1/2}) g_{2+}(\lambda) M'(k^s, v_1^{1/2})^* - \frac{(k^s)^2}{(2m)^2} M(k^s, |v_1|^{1/2}) g_{2+}(\lambda)$$
$$\times [v_1^{1/2}(H_1^0 - \lambda - i0)^{-1} A^* A (H_1^0 - \lambda - i0)^{-1} |v_1|^{1/2}] g_{2+}(\lambda) M(k^s, v_1^{1/2})^*$$
$$+ \frac{1}{2m} M(k^s, |v_1|^{1/2}) g_{2+}(\lambda) [v_1^{1/2}(H_1^0 - \lambda - i0)^{-1} A^* |v_2|^{1/2}]$$
$$\times [v_2^{1/2} A (H_1^0 - \lambda - i0)^{-1} |v_1|^{1/2}] g_{2+}(\lambda) M(k^s, v_1^{1/2})^*$$
$$- \frac{1}{2m} M(k^s, |v_1|^{1/2}) g_{2+}(\lambda) [v_1^{1/2}(H_1^0 - \lambda - i0)^{-1} A^* |v_2|^{1/2}] M(k^s, A^* v_2^{1/2})^*\Big\},$$
$$\lambda \in I_0. \tag{4.25}$$

Remark 4.3. Even though we may take $\mathscr{K}_j = \mathscr{H}_j$, $j = 1, 2$, $\mathscr{K} = \mathscr{H}$ for the applications we have in mind in Sect. 5, generalizations to singular interactions (of Yukawa-type) usually require the introduction of weighted L^2-spaces or certain Sobolev spaces, where $\mathscr{K}_j \subsetneqq \mathscr{H}_j$, $j = 1, 2$ (see e.g. [2, 19, 20, 26]). For completeness we included this generalization in Sects. 3 and 4.

Remark 4.4. Following the usual convention we have subtracted the rest energy mc^2 from $H^0(c)$ and then studied $I \subseteq \mathbb{R}^+$. Similarly one could add the rest energy and consider $I \subseteq (-\infty, 0)$.

Remark 4.5. For later purpose [see e.g. (5.40)] we note that Assumption 4.1 (ii) implies that

$$v_1^{1/2}(H_1^0 - \lambda - i0)^{-2}|v_1|^{1/2} = \frac{d}{d\lambda} v_1^{1/2}(H_1^0 - \lambda - i0)^{-1}|v_1|^{1/2}. \tag{4.26}$$

5. Applications

Finally, we illustrate the abstract result of Theorem 4.2 with the help of two concrete realizations: One-dimensional Dirac operators in Sect. 5.1 and three-dimensional ones in Sect. 5.2. General references on relativistic spectral and scattering theory relevant in the present context are [8, 15, 21, 25–27, 30, 34, 35, 39, 43].

5.1. The Dirac Operator in $L^2(\mathbb{R})^2$

The free Dirac operator $H^0(c)$ in $L^2(\mathbb{R})^2$ is defined by

$$H^0(c) := cp\sigma_1 + mc^2\sigma_3, \qquad m, c \in \mathbb{R}^+, \qquad \mathscr{D}(H^0(c)) = H^{2,1}(\mathbb{R})^2, \tag{5.1}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$
$$p := -i\frac{d}{dx}, \qquad \mathscr{D}(p) = H^{2,1}(\mathbb{R}). \tag{5.2}$$

Let V be the maximal multiplication operator with the real-valued function $v = v(x)$, and for some $\alpha > 0$ assume

$$e^{\alpha|\cdot|}v(\cdot) \in L^1(\mathbb{R}) \cap L^2(\mathbb{R}). \tag{5.3}$$

The Dirac operator $H(c)$ in $L^2(\mathbb{R})^2$ is then defined as

$$H(c) := H^0(c) + V, \qquad \mathscr{D}(H(c)) = \mathscr{D}(H^0(c)). \tag{5.4}$$

$H(c)$ is self-adjoint and

$$\sigma_{\text{ess}}(H(c)) = (-\infty, -mc^2] \cup [mc^2, \infty). \tag{5.5}$$

In order to prove this statement we note that $f \in H^{2,1}(\mathbb{R})$ implies $f \in L^\infty(\mathbb{R})$ and thus

$$\|vf\|_2 \leq \|v\|_2 \, \|f\|_\infty < \infty \quad \text{implying} \quad \mathscr{D}(p) \subseteq \mathscr{D}(V). \tag{5.6}$$

The integral kernel $k(x, y)$ of $V(H^0(c) - z)^{-1}$ is given by (see e.g. [13])

$$k(x,y) = v(x)e^{i\tilde{k}|x-y|}\frac{i}{2c}\begin{pmatrix} \tilde{k}_0^{-1} & \operatorname{sgn}(x-y) \\ \operatorname{sgn}(x-y) & \tilde{k}_0 \end{pmatrix},$$
$$z \in \mathbb{C}\backslash\{(-\infty, -mc^2] \cup [mc^2, \infty)\}, \tag{5.7}$$

$$c\tilde{k}(z) = (z^2 - m^2c^4)^{\frac{1}{2}}, \qquad \operatorname{Im}\tilde{k}(z) > 0, \qquad \tilde{k}_0(z) = \frac{c\tilde{k}(z)}{z + mc^2}. \tag{5.8}$$

This integral kernel is in $L^2(\mathbb{R}\times\mathbb{R})^2$ and therefore the potential V is relatively compact with respect to $H^0(c)$. Weyl's theorem [29, p. 112] then yields (5.5).

Subtracting the rest energy according to (3.1) we therefore identify

$$\mathscr{H}_1=\mathscr{H}_2=\mathscr{K}_1=\mathscr{K}_2=L^2(\mathbb{R}),\qquad I=\mathbb{R}^+,\qquad e=\emptyset,\qquad \mathscr{C}=\mathbb{C}^2,\tag{5.9}$$

$$A=A^*=p=-i\frac{d}{dx},\qquad \mathscr{D}(A)=H^{2,1}(\mathbb{R}),\tag{5.10}$$

$$\begin{aligned}&V_1=V_2=V,\qquad V=v^{1/2}|v|^{1/2},\qquad v^{1/2}=|v|^{1/2}\operatorname{sgn}(v),\\ &Y=Y^*=B(c)^{-1}|v|^{1/2},\qquad Z=Z^*=B(c)v^{1/2}.\end{aligned}\tag{5.11}$$

Then clearly Assumptions 3.1–3.3, 3.5, and 3.7 are satisfied. Assumption 3.6 follows from the explicit expression (5.18) and Assumption 3.7. Assumption 3.8 is clearly satisfied if $\operatorname{Ran}(|v|^{1/2})$ is dense in $L^2(\mathbb{R})$. This in turn is satisfied if $\operatorname{supp}(|v|^{1/2})=\mathbb{R}$. If $\operatorname{supp}(|v|^{1/2})\subsetneqq\mathbb{R}$ one simply replaces $|v|^{1/2}$ by $|\tilde v|^{1/2}$, where

$$|\tilde v(x)|^{1/2}:=\begin{cases}|v(x)|^{1/2}, & x\in\operatorname{supp}(v)\\ e^{-x^2}, & x\notin\operatorname{supp}(v),\end{cases}\tag{5.12}$$

since then $V=v^{1/2}|v|^{1/2}=v^{1/2}|\tilde v|^{1/2}$. Hence we always may assume $\operatorname{supp}(|v|^{1/2})=\mathbb{R}$ without loss of generality.

It remains to verify Assumption 4.1.

(i) Holomorphy of $Q_{1+}(\lambda,c)$, $\lambda>0$.

The integral kernel $q(x,y,\lambda,c)$ of

$$Q_{1+}(\lambda,c)=v^{1/2}B(c)\,(H^0(c)-mc^2-\lambda-i0)^{-1}B(c)^{-1}|v|^{1/2}\tag{5.13}$$

reads

$$\begin{aligned}&q(x,y,\lambda,c)=v(x)^{1/2}e^{ik|x-y|}\,\frac{i}{2}\begin{pmatrix}\dfrac{1}{ck_0} & \dfrac{1}{c^2}\operatorname{sgn}(x-y)\\ \operatorname{sgn}(x-y) & \dfrac{k_0}{c}\end{pmatrix}|v(y)|^{1/2},\\ &\qquad\lambda>0,\\ &k^d(\lambda,c)=k^s(\lambda)\left(1+\frac{\lambda}{2mc^2}\right)^{1/2},\qquad k^s(\lambda)=\sqrt{2m\lambda},\\ &\qquad k_0(\lambda,c)=\frac{k^s(\lambda)}{2mc}\left(1+\frac{\lambda}{2mc^2}\right)^{-1/2}.\end{aligned}\tag{5.14}$$

Define the compact set $M\subseteq\mathbb{C}$

$$M:=\left\{c^{-2}\in\mathbb{C}\,\middle|\,|c^{-2}|\le|c_0^{-2}|<\frac{2m}{\lambda}\text{ and }2|\operatorname{Im}k^d(\lambda,c)|\le k^s\frac{\lambda}{m|c_0^2|}\le\alpha\right\}.\tag{5.15}$$

Using

$$\begin{aligned}&|k^d|\le k^s\left(1+\frac{\lambda}{2m|c_0^2|}\right)^{1/2},\\ &\left|\frac{k_0}{c}\right|\le\frac{k^s}{2m|c_0^2|}\left(1-\frac{\lambda}{2m|c_0^2|}\right)^{-1/2},\\ &\left|\frac{1}{ck_0}\right|\le\frac{2m}{k^s}\left(1+\frac{\lambda}{2m|c_0^2|}\right)^{1/2},\end{aligned}\tag{5.16}$$

and a matrix norm $\|\cdot\|$ in $\mathbb{C}^2$ we get for $c^{-2} \in M$ the bound

$$\|q(x,y,\lambda,c)\| \leq \text{const}(\lambda,\alpha)\,|v(x)|^{1/2}|v(y)|^{1/2}e^{\frac{\alpha}{2}|x|}e^{\frac{\alpha}{2}|y|}. \tag{5.17}$$

For $c^{-2} \in M$ and fixed λ we have a family of uniformly bounded Hilbert Schmidt operators. Since the integral kernel $q(x,y,\lambda,c)$ is a holomorphic function of c^{-2} around $c^{-2}=0$ we get holomorphy of $Q_{1+}(\lambda,c)$ by (5.3) and (5.13).

(ii) Holomorphy of $T(\lambda,c,Y)$, $\lambda>0$.

The integral kernel $t(x,\lambda,c)$ of $T(\lambda,c,Y) : L^2(\mathbb{R})^2 \to \mathbb{C}^2$, is explicitly given by (see [30] and (4.12))

$$t(x,\lambda,c) = \frac{1}{\sqrt{4\pi}}\,\frac{1}{\sqrt{ck_0}}\,|v(x)|^{1/2}\begin{pmatrix} e^{-ik^d x} & \frac{k_0}{c}\,e^{-ik^d x} \\ e^{ik^d x} & -\frac{k_0}{c}\,e^{ik^d x}\end{pmatrix}, \tag{5.18}$$

$$\|t(x,\lambda,c)\| \leq \text{const}(\lambda,\alpha)|v(x)|^{1/2}e^{\frac{\alpha}{2}|x|}. \tag{5.19}$$

(We note that F maps $L^2(\mathbb{R})^2 \to L^2((0,\infty);\mathbb{C}^2)$, see [30].)

For $c^{-2} \in M$ this is also a family of uniformly bounded Hilbert Schmidt operators, with integral kernel holomorphic in c^{-2} and therefore $T(\lambda,c,Y)$ is holomorphic in c^{-2} around $c^{-2}=0$. The holomorphy of $T(\lambda,c,Z)^*$ follows analogously.

The operator U_0 that diagonalizes $A^*A = p^2$ is given by $U_0 : L^2(\mathbb{R}) \to L^2((0,\infty), d\mu; \mathbb{C}^2)$,

$$(U_0 f)(\mu) = \frac{1}{\sqrt{2}}\,\mu^{-1/4}\begin{pmatrix}(U_F f)(\sqrt{u}) \\ (U_F f)(-\sqrt{u})\end{pmatrix}, \qquad f \in L^2(\mathbb{R}), \tag{5.20}$$

with

$$(U_F f)(k) := s-\lim_{R\to\infty}\int_{|x|\leq R} dx\, e^{-ikx} f(x), \qquad f \in L^2(\mathbb{R}) \tag{5.21}$$

the Fourier transform in $L^2(\mathbb{R})$. Thus we get $M(k^d, |v|^{1/2}) : L^2(\mathbb{R}) \to \mathbb{C}^2$,

$$\begin{aligned} M(k^d,|v|^{1/2})f &= \frac{1}{\sqrt{2}}\,(k^d)^{-1/2}\begin{pmatrix}(U_F|v|^{1/2}f)(k^d) \\ (U_F|v|^{1/2}f)(-k^d)\end{pmatrix} \\ &= (k^d)^{-1/2}\,\frac{1}{\sqrt{4\pi}}\begin{pmatrix}\int_{-\infty}^{\infty} e^{-ik^d x}|v(x)|^{1/2}f(x)dx \\ \int_{-\infty}^{\infty} e^{ik^d x}|v(x)|^{1/2}f(x)dx\end{pmatrix} \\ &= (k^d)^{-1/2}\,\frac{1}{\sqrt{4\pi}}\begin{pmatrix}\langle |v|^{1/2}\psi_{01}(k^d), f\rangle \\ \langle |v|^{1/2}\psi_{02}(k^d), f\rangle\end{pmatrix}, \qquad f \in L^2(\mathbb{R}), \end{aligned} \tag{5.22}$$

where

$$\psi_{0j}(k^d,x) := e^{\varepsilon i k^d x}, \qquad \varepsilon := (-1)^{j+1}, \qquad j=1,2, \tag{5.23}$$

$\langle\cdot,\cdot\rangle$ denotes the scalar product in $L^2(\mathbb{R})$, and $M(k^d, A^*|v|^{1/2}) : L^2(\mathbb{R}) \to \mathbb{C}^2$,

$$M(k^d, A^*|v|^{1/2})f = (k^d)^{1/2}\,\frac{1}{\sqrt{4\pi}}\begin{pmatrix}\langle |v|^{1/2}\psi_{01}(k^d), f\rangle \\ -\langle |v|^{1/2}\psi_{02}(k^d), f\rangle\end{pmatrix}, \qquad f \in L^2(\mathbb{R}), \tag{5.24}$$

For the adjoint operators we get $M(k^d, v^{1/2})^* : \mathbb{C}^2 \to L^2(\mathbb{R})$,

$$(M(k^d, v^{1/2})^* h)(x) = (k^d)^{-1/2}\,\frac{1}{\sqrt{4\pi}}\,v(x)^{1/2}(e^{ik^d x}h_1 + e^{-ik^d x}h_2) \tag{5.25}$$

and $M(k^d, A^* v^{1/2})^* : \mathbb{C}^2 \to L^2(\mathbb{R})$,

$$(M(k^d, A^* v^{1/2})^* h)(x) = (k^d)^{1/2} \frac{1}{\sqrt{4\pi}} v(x)^{1/2} (e^{ik^d x} h_1 - e^{-ik^d x} h_2), \quad h = \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \in \mathbb{C}^2. \tag{5.26}$$

The physical solutions $\psi^s_{\pm j}$ of the Schrödinger equation are defined by the Fredholm (respectively Lippmann-Schwinger) equation

$$v^{1/2}\psi^s_{\pm j} := g_{2\pm}(\lambda) v^{1/2} \psi^s_{0j}, \qquad \psi^s_{0j}(k^s, x) := e^{\varepsilon i k^s x}, \qquad k^s = \sqrt{2m\lambda}, \quad \varepsilon = (-1)^{j+1}, \quad j = 1, 2, \quad \lambda > 0, \tag{5.27}$$

where $g_{2\pm}(\lambda)$ has been defined in (4.4). From Jost function techniques we know that $e_\pm = \emptyset$, implying that $g_{2\pm}(\lambda)$ in invertible for all $\lambda \in \mathbb{R}^+$ (see e.g. [9, 28]).

For the nonrelativistic limit we get from (4.24) the well known formula

$$\begin{aligned} S^{(0)}(\lambda) &= \begin{pmatrix} T^{l(0)}(\lambda) & R^{r(0)}(\lambda) \\ R^{l(0)}(\lambda) & T^{r(0)}(\lambda) \end{pmatrix} = 1 - 2\pi i 2m M(k^s, |v|^{1/2}) g_{2+}(\lambda) M(k^s, v^{1/2})^* \\ &= 1 + \frac{2m}{2ik^s} \begin{pmatrix} \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \\ \langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \end{pmatrix}, \\ &\lambda > 0, \end{aligned} \tag{5.28}$$

where $T^{l(0)}$, $R^{l(0)}$, $T^{r(0)}$, $R^{r(0)}$, denote the transmission and reflection coefficients from the left respectively right incidence.

We note that $\psi^s_{+1} = T^{(0)} f^s_+$, $\psi^s_{+2} = T^{(0)} f^s_-$, where $f^s_\pm$ are the Jost solutions in the notation of [9]. We also note that $\psi^s_{-2}(k^s, x) = \psi^s_{+1}(-k^s, x)$ and $\psi^s_{-1}(k^s, x) = \psi^s_{+2}(-k^s, x)$. One has e.g.,

$$\begin{aligned} \frac{1}{T^{l(0)}(\lambda)} &= 1 - \frac{2m}{2ik^s} \int_{\mathbb{R}} e^{-ik^s x} v(x) f^s_+(k^s, x) dx, \\ \frac{1}{T^{r(0)}(\lambda)} &= 1 - \frac{2m}{2ik^s} \int_{\mathbb{R}} e^{ik^s x} v(x) f^s_-(k^s, x) dx = \frac{1}{T^{l(0)}(\lambda)}, \\ \frac{R^{l(0)}(\lambda)}{T^{l(0)}(\lambda)} &= \frac{2m}{2ik^s} \int_{\mathbb{R}} e^{ik^s x} v(x) f^s_+(k^s, x) dx, \\ \frac{R^{r(0)}(\lambda)}{T^{r(0)}(\lambda)} &= \frac{2m}{2ik^s} \int_{\mathbb{R}} e^{-ik^s x} v(x) f^s_-(k^s, x) dx. \end{aligned} \tag{5.29}$$

Calculating the remaining terms on the right-hand side of (4.25) yields:

2nd term

$$\begin{aligned} &\frac{ik^s}{16m} \begin{pmatrix} \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \\ \langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \end{pmatrix} \\ &+ \frac{(k^s)^2}{8m} \begin{pmatrix} -\langle x|v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & -\langle x|v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \\ \langle x|v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & \langle x|v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \end{pmatrix}. \end{aligned} \tag{5.30}$$

3[rd] term

$$\frac{-i}{4m}\begin{pmatrix} \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}p\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}p\psi^s_{+2}(k^s)\rangle \\ -\langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}p\psi^s_{+1}(k^s)\rangle & -\langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}p\psi^s_{+2}(k^s)\rangle \end{pmatrix}$$
$$+\frac{ik^s}{4m}\begin{pmatrix} \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{01}(k^s)\rangle & -\langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{02}(k^s)\rangle \\ -\langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{01}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{02}(k^s)\rangle \end{pmatrix}. \tag{5.31}$$

We remark that the integral kernel of $v^{1/2}A(H^0_1-\lambda-i0)^{-1}|v|^{1/2}$ is given by

$$v^{1/2}A(H^0_1-\lambda-i0)^{-1}|v|^{1/2}(x,x') = \frac{i}{2}\,v(x)^{1/2}\operatorname{sgn}(x-x')\,e^{ik^s|x-x'|}|v(x')|^{1/2}. \tag{5.32}$$

4[th] term

$$-\frac{ik^s}{4m}\begin{pmatrix} \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{01}(k^s)\rangle & -\langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{02}(k^s)\rangle \\ -\langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{01}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{02}(k^s)\rangle \end{pmatrix}. \tag{5.33}$$

5[th] term

$$\frac{ik^s}{16m}\begin{pmatrix} \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \\ \langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{02}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \end{pmatrix}$$
$$+\frac{(k^s)^2}{8m}\begin{pmatrix} \langle |v|^{1/2}\psi^s_{-1}(k^s), xv^{1/2}\psi^s_{01}(k^s)\rangle & -\langle |v|^{1/2}\psi^s_{-1}(k^s), xv^{1/2}\psi^s_{02}(k^s)\rangle \\ \langle |v|^{1/2}\psi^s_{-2}(k^s), xv^{1/2}\psi^s_{01}(k^s)\rangle & -\langle |v|^{1/2}\psi^s_{-2}(k^s), xv^{1/2}\psi^s_{02}(k^s)\rangle \end{pmatrix}. \tag{5.34}$$

6[th] term

$$\frac{ik^s}{8m^2}\begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}, \tag{5.35}$$

where

$$\begin{aligned} m_{11} &= \langle |v|^{1/2}\psi^s_{-1}(k^s), v^{1/2}(H^0_1-\lambda-i0)^{-1}p^2(H^0_1-\lambda-i0)^{-1}|v|^{1/2}v^{1/2}\psi^s_{+1}(k^s)\rangle, \\ m_{12} &= \langle |v|^{1/2}\psi^s_{-1}(k^s), v^{1/2}(H^0_1-\lambda-i0)^{-1}p^2(H^0_1-\lambda-i0)^{-1}|v|^{1/2}v^{1/2}\psi^s_{+2}(k^s)\rangle, \\ m_{21} &= \langle |v|^{1/2}\psi^s_{-2}(k^s), v^{1/2}(H^0_1-\lambda-i0)^{-1}p^2(H^0_1-\lambda-i0)^{-1}|v|^{1/2}v^{1/2}\psi^s_{+1}(k^s)\rangle, \\ m_{22} &= \langle |v|^{1/2}\psi^s_{-2}(k^s), v^{1/2}(H^0_1-\lambda-i0)^{-1}p^2(H^0_1-\lambda-i0)^{-1}|v|^{1/2}v^{1/2}\psi^s_{+2}(k^s)\rangle. \end{aligned} \tag{5.36}$$

7[th] term

$$\frac{-i}{4mk^s}\begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix}, \tag{5.37}$$

where

$$\begin{aligned} n_{11} &= \langle |v|^{1/2}p(\psi^s_{-1}(k^s)-\psi^s_{01}(k^s)), v^{1/2}p(\psi^s_{+1}(k^s)-\psi^s_{01}(k^s))\rangle, \\ n_{12} &= \langle |v|^{1/2}p(\psi^s_{-1}(k^s)-\psi^s_{01}(k^s)), v^{1/2}p(\psi^s_{+2}(k^s)-\psi^s_{02}(k^s))\rangle, \\ n_{21} &= \langle |v|^{1/2}p(\psi^s_{-2}(k^s)-\psi^s_{02}(k^s)), v^{1/2}p(\psi^s_{+1}(k^s)-\psi^s_{01}(k^s))\rangle, \\ n_{22} &= \langle |v|^{1/2}p(\psi^s_{-2}(k^s)-\psi^s_{02}(k^s)), v^{1/2}p(\psi^s_{+2}(k^s)-\psi^s_{02}(k^s))\rangle, \end{aligned} \tag{5.38}$$

8[th] term

$$\frac{-i}{4m}\begin{pmatrix} \langle |v|^{1/2}p(\psi^s_{-1}(k^s)-\psi^s_{01}(k^s)), v^{1/2}\psi^s_{01}(k^s)\rangle & -\langle |v|^{1/2}p(\psi^s_{-1}(k^s)-\psi^s_{01}(k^s)), v^{1/2}\psi^s_{02}(k^s)\rangle \\ \langle |v|^{1/2}p(\psi^s_{-2}(k^s)-\psi^s_{02}(k^s)), v^{1/2}\psi^s_{01}(k^s)\rangle & -\langle |v|^{1/2}p(\psi^s_{-2}(k^s)-\psi^s_{02}(k^s)), v^{1/2}\psi^s_{02}(k^s)\rangle \end{pmatrix}. \tag{5.39}$$

Using (4.26) we get

$$\begin{aligned} &ik^s\langle |v|^{1/2}\psi^s_{-1}(k^s), [v^{1/2}(H^0_1-\lambda-i0)^{-2}|v|^{1/2}]v^{1/2}\psi^s_{+1}(k^s)\rangle \\ &\quad = -m\langle |v|^{1/2}\psi^s_{-1}(k^s), xv^{1/2}\psi^s_{01}(k^s)\rangle + m\langle x|v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle \\ &\quad\quad - ik^s\frac{d}{d\lambda}\langle |v|^{1/2}\psi^s_{01}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle . \end{aligned} \tag{5.40}$$

Summing up we get for the first order correction term of order c^{-2} of the scattering matrix (in terms of transmission and reflection coefficients)

$$\begin{aligned} S^{(1)}(\lambda) &=: \begin{pmatrix} T^{l(1)}(\lambda) & R^{r(1)}(\lambda) \\ R^{l(1)}(\lambda) & T^{r(1)}(\lambda) \end{pmatrix} = \frac{(k^s)^4}{8m^3}\frac{dS^{(0)}(\lambda)}{d\lambda} \\ &+\frac{1}{4imk^s}\begin{pmatrix} \langle |v|^{1/2}p\psi^s_{-1}(k^s), v^{1/2}p\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}p\psi^s_{-1}(k^s), v^{1/2}p\psi^s_{+2}(k^s)\rangle \\ \langle |v|^{1/2}p\psi^s_{-2}(k^s), v^{1/2}p\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}p\psi^s_{-2}(k^s), v^{1/2}p\psi^s_{+2}(k^s)\rangle \end{pmatrix} \\ &+\frac{k^s}{4im}\begin{pmatrix} \langle |v|^{1/2}\psi^s_{-1}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{-1}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \\ \langle |v|^{1/2}\psi^s_{-2}(k^s), v^{1/2}\psi^s_{+1}(k^s)\rangle & \langle |v|^{1/2}\psi^s_{-2}(k^s), v^{1/2}\psi^s_{+2}(k^s)\rangle \end{pmatrix}, \quad \lambda>0. \end{aligned} \tag{5.41}$$

5.2. *The Dirac Operator in* $L^2(\mathbb{R}^3)^4$

The free Dirac operator $H^0(c)$ in $L^2(\mathbb{R}^3)^4$ is defined by:

$$H^0(c) := c\boldsymbol{\alpha}\mathbf{p} + \beta mc^2, \qquad m, c\in\mathbb{R}^+, \qquad \mathscr{D}(H^0(c)) = H^{2,1}(\mathbb{R}^3)^4, \tag{5.42}$$

where

$$\begin{gathered} \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\ \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\ \boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3), \qquad \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3), \\ \mathbf{p} := -i\nabla, \qquad \mathscr{D}(\mathbf{p}) = H^{2,1}(\mathbb{R}^3). \end{gathered} \tag{5.43}$$

Define (cf. e.g. [40, p. 305])

$$\begin{aligned} M_{v,\varrho}(x) &:= \left\{ \int_{|x-y|\le 1} d^3y|v(y)|^2|x-y|^{\varrho-3} \right\}^{1/2}, \qquad v \text{ measurable}, \qquad \varrho<3, \\ M_\varrho(\mathbb{R}^3) &:= \{v \mid M_{v,\varrho}(\cdot) \text{ bounded}\}, \end{aligned} \tag{5.44}$$

$$N_v(x) := \left\{ \int_{|x-y|\le 1} d^3y|v(y)|^2 \right\}^{1/2}, \quad \text{for all } x\in\mathbb{R}^3, \quad \text{and } v\in L^2_{\text{loc}}(\mathbb{R}^3), \tag{5.45}$$

and let V be the maximal operator of multiplication with the real-valued function $v = v(x)$ where

$$v \in M_\varrho(\mathbb{R}^3) \text{ for some } \varrho < 2. \tag{5.46}$$

$$v \in L^1(\mathbb{R}^3). \tag{5.47}$$

$$ve^{\alpha|\cdot|} \quad \text{fullfills (5.46) and (5.47) for some } \alpha > 0. \tag{5.48}$$

The Dirac operator $H(c)$ in $L^2(\mathbb{R}^3)^4$ is now defined as

$$H(c) := H^0(c) + V, \qquad \mathscr{D}(H(c)) = \mathscr{D}(H^0(c)). \tag{5.49}$$

The hypotheses (5.46)–(5.48) then imply
(i) V is $H^0(c)$ bounded with relative bound 0 by (5.46) (see [40, Theorem 10.18]).
(ii) Since $v \in M_\varrho(\mathbb{R}^3)$ with $\varrho < 2$ it follows that $v^{1/2} \in M_\sigma(\mathbb{R}^3)$ with $\sigma < 1$ and $M_\sigma(\mathbb{R}^3) \subseteq M_\varrho(\mathbb{R}^3)$, $\sigma \le \varrho$.

Since $v^{1/2} \in L^2(\mathbb{R}^3)$ we have $N_{v^{1/2}}(x) \to 0$ for $|x| \to \infty$.

Thus $V^{1/2}$ is $H^0(c)$ compact (cf. [40, Auxiliary Theorem 10.24 and Theorem 10.21]).

Subtracting the rest energy according to (3.1) we therefore identify:

$$\begin{gathered}\mathscr{H}_1 = \mathscr{H}_2 = \mathscr{K}_1 = \mathscr{K}_2 = L^2(\mathbb{R}^3)^2, \\ I = \mathbb{R}^+, \qquad I_{\pm 0} = I \backslash e_\pm(c^{-2} = 0), \qquad \mathscr{C} = L^2(S^2)^2,\end{gathered} \tag{5.50}$$

$$\begin{gathered}A = A^* = \begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix}, \qquad \mathscr{D}(A) = H^{2,1}(\mathbb{R}^3)^2, \\ p_j = -i\frac{\partial}{\partial x_j}, \qquad j = 1,2,3,\end{gathered} \tag{5.51}$$

$$\begin{gathered}V_1 = V_2 = V, \qquad V = v^{1/2}|v|^{1/2}, \qquad v^{1/2} = |v|^{1/2}\operatorname{sgn}(v), \\ Y = Y^* = B(c)^{-1}|v|^{1/2}, \qquad Z = Z^* = B(c)v^{1/2}.\end{gathered} \tag{5.52}$$

(Here S^2 denotes the unit sphere in $\mathbb{R}^3$.) Due to our hypothesis (5.48), $e(c)$ is a discrete set [26].

Clearly Assumptions 3.1–3.3, 3.5 and 3.7 are satisfied. Assumption 3.6 follows from the explicit expression (5.60) and Assumption 3.7. Assumption 3.8 can be dealt with in exactly the same way as in Sect. 5.1. It remains to verify Assumption 4.1.

(i) Holomorphy of $Q_{1+}(\lambda, c)$, $\lambda \in I_{+0}$.

The integral kernel $q(x, y, \lambda, c)$ of

$$Q_{1+}(\lambda, c) = v^{1/2}B(c)\,(H^0(c) - mc^2 - \lambda - i0)^{-1}B(c)^{-1}|v|^{1/2} \tag{5.53}$$

is given by

$$q(x, y, \lambda, c) = v(x)^{1/2}\,\frac{e^{ik^d|x-y|}}{|x-y|}\,\frac{1}{4\pi}\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44}\end{pmatrix}|v(y)|^{1/2}, \tag{5.54}$$

$$\begin{aligned}
&a_{11} = a_{22} = \frac{\lambda}{c^2} + 2m, \qquad a_{33} = a_{44} = \frac{\lambda}{c^2}, \qquad a_{12} = a_{21} = a_{34} = a_{43} = 0,\\
&a_{13} = \frac{a}{c^2}\,(x_3 - y_3), \qquad a_{14} = \frac{a}{c^2}\,[(x_1 - y_1) - i(x_2 - y_2)],\\
&a_{23} = \frac{a}{c^2}\,[(x_1 - y_1) + i(x_2 - y_2)] \qquad a_{24} = -\frac{a}{c^2}\,(x_3 - y_3),\\
&a_{31} = a(x_3 - y_3), \qquad a_{32} = a[(x_1 - y_1) - i(x_2 - y_2)],\\
&a_{41} = a[(x_1 - y_1) + i(x_2 - y_2)], \qquad a_{42} = -a(x_3 - y_3),\\
&\lambda \in I_{+0}, \qquad k^d(\lambda, c) = k^s\left(1 + \frac{\lambda}{2mc^2}\right)^{1/2}, \qquad k^s = \sqrt{2m\lambda},
\end{aligned} \tag{5.55}$$

where

$$a(x,y) := |x-y|^{-2}(k^d|x-y|+i), \qquad x,y \in \mathbb{R}^3, \qquad x \neq y. \tag{5.56}$$

Define the compact set $M \subseteq \mathbb{C}$

$$M := \left\{ c^{-2} \in \mathbb{C} \,\middle|\, |c^{-2}| \leq |c_0^{-2}| < \frac{2m}{\lambda} \text{ and } 2|\operatorname{Im} k^d(\lambda,c)| \leq k^s \frac{\lambda}{m|c_0^2|} \leq \alpha \right\}. \tag{5.57}$$

Using

$$|k^d| \leq k^s \left(1 + \frac{\lambda}{2m|c_0^2|}\right)^{1/2} \tag{5.58}$$

and a matrix norm $\|\cdot\|$ in $\mathbb{C}^4$ we get for $c^{-2} \in M$ the bound (cf. [8])

$$\|q(x,y,\lambda,c)\| \leq \operatorname{const}(\lambda,\alpha)|v(x)|^{1/2}|v(y)|^{1/2} e^{\frac{\alpha}{2}|x|} e^{\frac{\alpha}{2}|y|} \left(\frac{1}{|x-y|} + \frac{1}{|x-y|^2}\right). \tag{5.59}$$

For $c^{-2} \in M$ and fixed λ we have a family of uniformly bounded operators (using [40, Theorem 6.24], the fact that $v^{1/2}e^{\frac{\alpha}{2}|\cdot|} \in M_\sigma$, $\sigma < 1$ and $v^{1/2}e^{\frac{\alpha}{2}|\cdot|} \in L^2(\mathbb{R}^3)$). Since the integral kernel $q(x,y,\lambda,c)$ is a holomorphic function of c^{-2} around $c^{-2} = 0$ we get holomorphy of $Q_{1+}(\lambda,c)$.

(ii) Holomorphy of $T(\lambda,c,Y)$, $\lambda > 0$.

The integral kernel $t(x,\lambda,c,\omega)$ of $T(\lambda,c,Y) : L^2(\mathbb{R}^3)^4 \to L^2(S^2)^2$ is given by (see [34] and (4.12))

$$\begin{aligned} t(x,\lambda,c,\omega) &= (2\pi)^{-3/2}\sqrt{\frac{k^d}{2}}\sqrt{\frac{\lambda+2mc^2}{c^2}}\, e^{-ik^d\omega x}|v(x)|^{1/2} \\ &\times \begin{pmatrix} 1 & 0 & \frac{k_0}{c}\,\omega_3 & \frac{k_0}{c}(\omega_1 - i\omega_2) \\ 0 & 1 & \frac{k_0}{c}(\omega_1 + i\omega_2) & -\frac{k_0}{c}\,\omega_3 \end{pmatrix}, \\ k_0 &= \sqrt{\frac{\lambda}{\lambda+2mc^2}}, \qquad \omega \in S^2. \end{aligned} \tag{5.60}$$

(We note that F maps $L^2(\mathbb{R}^3)^4 \to L^2((0,\infty); L^2(S^2)^2)$ (see [34]).) For $\lambda \in I$ we get

$$\|t(\omega,x,\lambda,c)\| \leq \operatorname{const}(\lambda,\alpha)|v(x)|^{1/2} e^{\frac{\alpha}{2}|x|}. \tag{5.61}$$

For $c^{-2} \in M$ this is also a family of uniformly bounded Hilbert Schmidt operators (since $ve^{\alpha|\cdot|} \in L^1(\mathbb{R}^3)$, with integral kernel holomorphic in c^{-2} and therefore $T(\lambda,c,Y)$ is holomorphic in c^{-2} around $c^{-2} = 0$.

The holomorphy of $T(\lambda,c,Z)^*$ follows similarly.

In particular, $S(\lambda,c) - 1$ is a trace class operator, i.e.,

$$[S(\lambda,c) - 1] \in \mathscr{B}_1(L^2(S^2)^2), \qquad \lambda \in I \backslash e_+(c). \tag{5.62}$$

The operator U_0 that diagonalizes A^*A is given by $U_0 : L^2(\mathbb{R}^3)^2 \to L^2((0,\infty), d\mu; L^2(S^2)^2)$,

$$\begin{aligned} (U_0 f)(\mu,\omega))_j &= \frac{1}{\sqrt{2}}\mu^{1/4}(U_F f_j)(\sqrt{\mu}\omega), \\ j &= 1,2, \qquad \omega \in S^2, \qquad f \in L^2(\mathbb{R}^3)^2, \end{aligned} \tag{5.63}$$

with

$$(U_F f)(k\omega) := s - \lim_{R\to\infty} \int\limits_{|x|\leq R} d^3x\, e^{-ik\omega x} f(x),$$
$$f \in L^2(R^3), \qquad k = \sqrt{\mu}, \qquad k > 0, \tag{5.64}$$

the Fourier transform in $L^2(\mathbb{R}^3)$.

Thus we get $M(k^d, |v|^{1/2}) : L^2(\mathbb{R}^3)^2 \to L^2(S^2)^2$,

$$\begin{aligned}
&(M(k^d, |v|^{1/2})f)(\omega)_j \\
&= \frac{1}{\sqrt{2}} (k^d)^{1/2} (U_F |v|^{1/2} f_j)(k^d\omega) \\
&= \frac{1}{\sqrt{2}} (k^d)^{1/2} (2\pi)^{-3/2} \int\limits_{\mathbb{R}^3} d^3x\, e^{-ik^d\omega x} |v(x)|^{1/2} f_j(x) \\
&= \frac{1}{\sqrt{2}} (k^d)^{1/2} (2\pi)^{-3/2} \langle |v|^{1/2} \psi_0(k^d\omega), f_i\rangle, \quad f_j \in L^2(\mathbb{R}^3), \quad j = 1,2,
\end{aligned} \tag{5.65}$$

where $\psi_0(k^d\omega, x) := e^{ik^d\omega x}$ and $\langle\cdot,\cdot\rangle$ now denotes the scalar product in $L^2(\mathbb{R}^3)$.

Similarly we have $M(k^d, A^*|v|^{1/2}) : L^2(\mathbb{R}^3)^2 \to L^2(S^2)^2$,

$$\begin{aligned}
&(M(k^d, A^*|v|^{1/2})f)(\omega) \\
&= \frac{1}{\sqrt{2}} (k^d)^{3/2} (2\pi)^{-3/2} \begin{pmatrix} \omega_3 & \omega_1 - i\omega_2 \\ \omega_1 + i\omega_2 & -\omega_3 \end{pmatrix} \\
&\times \begin{pmatrix} \langle |v|^{1/2}\psi_0(k^d\omega), f_3\rangle \\ \langle |v|^{1/2}\psi_0(k^d\omega), f_4\rangle \end{pmatrix}, \qquad f \in L^2(\mathbb{R}^3)^2.
\end{aligned} \tag{5.66}$$

For the corresponding adjoint operators we obtain $M(k^d, v^{1/2})^* : L^2(S^2)^2 \to L^2(\mathbb{R}^3)^2$,

$$(M(k^d, v^{1/2})^* h)(x)_j = \frac{1}{\sqrt{2}} (k^d)^{1/2} (2\pi)^{-3/2} v(x)^{1/2} \int\limits_{S^2} d\omega\, e^{ik^d\omega x} h_j(\omega),$$
$$h_j \in L^2(S^2), \qquad j = 1,2, \tag{5.67}$$

and $M(k^d, A^* v^{1/2})^* : L^2(S^2)^2 \to L^2(\mathbb{R}^3)^2$,

$$\begin{aligned}
&(M(k^d, A^* v^{1/2})^* h)(x) \\
&= \frac{1}{\sqrt{2}} (k^d)^{3/2} (2\pi)^{-3/2} v(x)^{1/2} \int\limits_{S^2} d\omega \begin{pmatrix} \omega_3 & (\omega_1 - i\omega_2) \\ (\omega_1 + i\omega_2) & -\omega_3 \end{pmatrix} \\
&\times \begin{pmatrix} h_1(\omega) \\ h_2(\omega) \end{pmatrix} e^{ik^d\omega x}, \qquad h \in L^2(S^2)^2.
\end{aligned} \tag{5.68}$$

The physical solutions $\psi_\pm^s$ of the Schrödinger (Pauli) equation are defined by the Fredholm (respectively Lippmann-Schwinger) equation (see e.g. [1, 28])

$$v^{1/2}\psi_\pm^s(k^s\omega) := g_{2\pm}(\lambda) v^{1/2} \psi_0^s(k^s\omega), \qquad \psi_0^s(k^s\omega, x) = e^{ik^s\omega x},$$
$$k^s = \sqrt{2m\lambda}, \qquad \lambda \in I_{\pm 0}, \qquad \omega \in S^2. \tag{5.69}$$

For the nonrelativistic limit $S^{(0)}(\lambda)$ we get from (4.24) the well known result [1, 3, 4, 22, 24, 28]

$$
\begin{aligned}
(S^{(0)}(\lambda)h)(\omega)_j &= ([1-2\pi i 2mM(k^s,|v|^{1/2})g_{2+}(\lambda)M(k^s,v^{1/2})^*]h)(\omega)_j \\
&= h_j(\omega) - 2\pi i \frac{k^s}{2} 2m(2\pi)^{-3} \int_{\mathbb{R}^3} d^3x\, e^{-ik^s\omega x}|v(x)|^{1/2} \\
&\quad \times g_{2+}(\lambda) v^{1/2}(\cdot) \int_{S^2} d\omega'\, e^{ik^s\omega'(\cdot)} h_j(\omega') \\
&= h_j(\omega) - imk^s(2\pi)^{-2} \int_{S^2} d\omega' h_j(\omega') \langle |v|^{1/2}\psi_0^s(k^s\omega), v^{1/2}\psi_+^s(k^s\omega')\rangle, \\
&\quad h_j \in L^2(S^2), \qquad j=1,2, \qquad \text{a.e. } \lambda \in I. \qquad (5.70)
\end{aligned}
$$

Calculating the remaining terms on the right-hand side of (4.25) yields:

2nd term

$$
\begin{aligned}
&-\frac{i(k^s)^3}{16m}(2\pi)^{-2} \int_{S^2} d\omega' \langle |v|^{1/2}\psi_0^s(k^s\omega), v^{1/2}\psi_+^s(k^s\omega')\rangle h_j(\omega') \\
&-\frac{(k^s)^4}{8m}(2\pi)^{-2} \int_{S^2} d\omega' \langle |v|^{1/2}(\omega\cdot x)\psi_0^s(k^s\omega), v^{1/2}\psi_+^s(k^s\omega')\rangle h_j(\omega'), \qquad j=1,2.
\end{aligned} \qquad (5.71)
$$

3rd term

$$
\frac{i(k^s)^2}{4m}(2\pi)^{-2} \int_{S^2} d\omega' \begin{pmatrix} b_1(\omega,\omega') \\ b_2(\omega,\omega') \end{pmatrix}, \qquad (5.72)
$$

where

$$
\begin{aligned}
b_1(\omega,\omega') &= \langle |v|^{1/2}\psi_0^s(k^s\omega), \omega_3 v^{1/2}[p_3(\psi_0^s(k^s\omega') \\
&\quad - \psi_+^s(k^s\omega'))h_1(\omega') + (p_1 - ip_2)(\psi_0^s(k^s\omega') - \psi_+^s(k^s\omega'))h_2(\omega')]\rangle \\
&\quad + \langle |v|^{1/2}\psi_0^s(k^s\omega), (\omega_1 - i\omega_2) v^{1/2}[(p_1+ip_2)(\psi_0^s(k^s\omega') \\
&\quad - \psi_+^s(k^s\omega'))h_1(\omega') - p_3(\psi_0^s(k^s\omega') - \psi_+^s(k^s\omega'))h_2(\omega')]\rangle, \\
b_2(\omega,\omega') &= \langle |v|^{1/2}\psi_0^s(k^s\omega), (\omega_1 + i\omega_2) v^{1/2}[p_3(\psi_0^s(k^s\omega') \\
&\quad - \psi_+^s(k^s\omega'))h_1(\omega') + (p_1 - ip_2)(\psi_0^s(k^s\omega') - \psi_+^s(k^s\omega'))h_2(\omega')]\rangle \\
&\quad - \langle |v|^{1/2}\psi_0^s(k^s\omega), \omega_3 v^{1/2}[(p_1+ip_2)(\psi_0^s(k^s\omega') \\
&\quad - \psi_+^s(k^s\omega'))h_1(\omega') - p_3(\psi_0^s(k^s\omega') - \psi_+^s(k^s\omega'))h_2(\omega')]\rangle.
\end{aligned} \qquad (5.73)
$$

4th term

$$
\begin{aligned}
&-\frac{i(k^s)^3}{4m}(2\pi)^{-2} \int_{S^2} d\omega' \langle |v|^{1/2}\psi_0^s(k^s\omega), v^{1/2}\psi_0^s(k^s\omega')\rangle \\
&\times \begin{pmatrix} \omega_3\omega_3' + (\omega_1 - i\omega_2)(\omega_1' + i\omega_2') & \omega_3(\omega_1' - i\omega_2') - (\omega_1 - i\omega_2)\omega_3' \\ (\omega_1 + i\omega_2)\omega_3' - \omega_3(\omega_1' + i\omega_2') & (\omega_1 + i\omega_2)(\omega_1' - i\omega_2') + \omega_3\omega_3' \end{pmatrix} \\
&\times \begin{pmatrix} h_1(\omega') \\ h_2(\omega') \end{pmatrix}.
\end{aligned} \qquad (5.74)
$$

5^{th} term

$$\begin{aligned}&-\frac{i(k^s)^3}{16m}(2\pi)^{-2}\int_{S^2}d\omega'\langle|v|^{1/2}\psi_0^s(k^s\omega),v^{1/2}\psi_+^s(k^s\omega')\rangle h_j(\omega')\\&+\frac{(k^s)^4}{8m}(2\pi)^{-2}\int_{S^2}d\omega'\langle|v|^{1/2}\psi_-^s(k^s\omega),v^{1/2}(\omega'\cdot x)\psi_0^s(k^s\omega')\rangle h_j(\omega'),\quad j=1,2.\end{aligned}\tag{5.75}$$

6^{th} term

$$\begin{aligned}&\frac{i(k^s)^3}{4m}(2\pi)^{-2}\int_{S^2}d\omega'\langle|v|^{1/2}(\psi_0^s(k^s\omega)-\psi_-^s(k^s\omega)),v^{1/2}\psi_+^s(k^s\omega')\rangle h_j(\omega')\\&+\frac{i(k^s)^5}{8m^2}(2\pi)^{-2}\int_{S^2}d\omega'\langle|v|^{1/2}\psi_-^s(k^s\omega),[v^{1/2}(H_1^0-\lambda-i0)^{-2}|v|^{1/2}]\\&\quad\times v^{1/2}\psi_+^s(k^s\omega')\rangle h_j(\omega'),\quad j=1,2.\end{aligned}\tag{5.76}$$

7^{th} term

$$-\frac{ik^s}{4m}(2\pi)^{-2}\int_{S^2}d\omega'\begin{pmatrix}d_1(\omega,\omega')\\d_2(\omega,\omega')\end{pmatrix},\tag{5.77}$$

where

$$\begin{aligned}d_1(\omega,\omega')&=\langle|v|^{1/2}p_3(\psi_0^s(k^s\omega)-\psi_-^s(k^s\omega)),v^{1/2}[p_3(\psi_0^s(k^s\omega')\\&\quad-\psi_+^s(k^s\omega'))h_1(\omega')+(p_1-ip_2)(\psi_0^s(k^s\omega')-\psi_+^s(k^s\omega'))h_2(\omega')]\rangle\\&\quad+\langle|v|^{1/2}(p_1+ip_2)(\psi_0^s(k^s\omega)-\psi_-^s(k^s\omega)),v^{1/2}[(p_1+ip_2)(\psi_0^s(k^s\omega')\\&\quad-\psi_+^s(k^s\omega'))h_1(\omega')-p_3(\psi_0^s(k^s\omega')-\psi_+^s(k^s\omega'))h_2(\omega')]\rangle,\\d_2(\omega,\omega')&=\langle|v|^{1/2}(p_1-ip_2)(\psi_0^s(k^s\omega)-\psi_-^s(k^s\omega)),v^{1/2}[p_3(\psi_0^s(k^s\omega')\\&\quad-\psi_+^s(k^s\omega'))h_1(\omega')+(p_1-ip_2)(\psi_0^s(k^s\omega')-\psi_+^s(k^s\omega'))h_2(\omega')]\rangle\\&\quad-\langle|v|^{1/2}p_3(\psi_0^s(k^s\omega)-\psi_-^s(k^s\omega)),v^{1/2}[(p_1+ip_2)(\psi_0^s(k^s\omega')\\&\quad-\psi_+^s(k^s\omega'))h_1(\omega')-p_3(\psi_0^s(k^s\omega')-\psi_+^s(k^s\omega'))h_2(\omega')]\rangle.\end{aligned}\tag{5.78}$$

In order to simplify (5.78) one can use

$$\langle|v|^{1/2}\boldsymbol{\sigma}\mathbf{p}\psi_-^s(k^s\omega),v^{1/2}\boldsymbol{\sigma}\mathbf{p}\psi_+^s(k^s\omega')\rangle=\begin{pmatrix}a_{11}(\omega,\omega')&a_{12}(\omega,\omega')\\a_{21}(\omega,\omega')&a_{22}(\omega,\omega')\end{pmatrix},\tag{5.79}$$

where

$$\begin{aligned}a_{11}(\omega,\omega')&=\langle|v|^{1/2}p_3\psi_-^s(k^s\omega),v^{1/2}p_3\psi_+^s(k^s\omega')\rangle\\&\quad+\langle|v|^{1/2}(p_1+ip_2)\psi_-^s(k^s\omega),v^{1/2}(p_1+ip_2)\psi_+^s(k^s\omega')\rangle,\end{aligned}\tag{5.80}$$

$$\begin{aligned}a_{12}(\omega,\omega')&=\langle|v|^{1/2}p_3\psi_-^s(k^s\omega),v^{1/2}(p_1-ip_2)\psi_+^s(k^s\omega')\rangle\\&\quad-\langle|v|^{1/2}(p_1+ip_2)\psi_-^s(k^s\omega),v^{1/2}p_3\psi_+^s(k^s\omega')\rangle,\end{aligned}\tag{5.81}$$

$$\begin{aligned}a_{21}(\omega,\omega')&=\langle|v|^{1/2}(p_1-ip_2)\psi_-^s(k^s\omega),v^{1/2}p_3\psi_+^s(k^s\omega')\rangle\\&\quad-\langle|v|^{1/2}p_3\psi_-^s(k^s\omega),v^{1/2}(p_1+ip_2)\psi_+^s(k^s\omega')\rangle,\end{aligned}\tag{5.82}$$

$$\begin{aligned}a_{22}(\omega,\omega')&=\langle|v|^{1/2}(p_1-ip_2)\psi_-^s(k^s\omega),v^{1/2}(p_1-ip_2)\psi_+^s(k^s\omega')\rangle\\&\quad+\langle|v|^{1/2}p_3\psi_-^s(k^s\omega),v^{1/2}p_3\psi_+^s(k^s\omega')\rangle,\end{aligned}\tag{5.83}$$

8^{th} term

$$\frac{i(k^s)^2}{4m}(2\pi)^{-2}\int_{S^2} d\omega'$$

$$\times\left[\begin{pmatrix} \langle |v|^{1/2}p_3(\psi_0^s(k^s\omega)-\psi_-^s(k^s\omega)), v^{1/2}\psi_0^s(k^s\omega')\rangle[\omega_3' h_1(\omega')+(\omega_1'-i\omega_2')h_2(\omega')] \\ \langle |v|^{1/2}(p_1-ip_2)(\psi_0^s(k^s\omega)-\psi_-^s(k^s\omega)), v^{1/2}\psi_0^s(k^s\omega')\rangle[\omega_3' h_1(\omega')+(\omega_1'-i\omega_2')h_2(\omega')] \end{pmatrix}\right.$$

$$\left.+\begin{pmatrix} \langle |v|^{1/2}(p_1+ip_2)(\psi_0^s(k^s\omega)-\psi_-^s(k^s\omega)), v^{1/2}\psi_0^s(k^s\omega')\rangle[(\omega_1'+i\omega_2')h_1(\omega')-\omega_3' h_2(\omega')] \\ -\langle |v|^{1/2}p_3(\psi_0^s(k^s\omega)-\psi_-^s(k^s\omega)), v^{1/2}\psi_0^s(k^s\omega')\rangle[(\omega_1'+i\omega_2')h_1(\omega')-\omega_3' h_2(\omega')] \end{pmatrix}\right]. \tag{5.84}$$

Summing up we get for the first order correction term in c^{-2} of the scattering matrix

$$\begin{aligned}(S^{(1)}(\lambda)h)(\omega) &= \frac{(k^s)^4}{8m^3}\left(\frac{d(S^{(0)}(\lambda)}{d\lambda}h\right)(\omega) \\ &+(2\pi)^{-2}\int_{S^2} d\omega'\left[\frac{(k^s)^3}{4im}\langle |v|^{1/2}\psi_-^s(k^s\omega), v^{1/2}\psi_+^s(k^s\omega')\rangle 1\right. \\ &\left.+\frac{k^s}{4im}\langle |v|^{1/2}\boldsymbol{\sigma}\mathbf{p}\psi_-^s(k^s\omega), v^{1/2}\boldsymbol{\sigma}\mathbf{p}\psi_+^s(k^s\omega')\rangle\right]\begin{pmatrix} h_1(\omega') \\ h_2(\omega')\end{pmatrix}, \\ &\text{a.e. } \lambda\in I, \quad \omega\in S^2, \quad h=\begin{pmatrix} h_1 \\ h_2\end{pmatrix}\in L^2(S^2)^2. \end{aligned} \tag{5.85}$$

The analogous expansion of the scattering amplitude up to order $O(c^{-2})$ can be found in Appendix A.

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Appendix A. Comparison with the Foldy-Wouthuysen Method

In this appendix we compare our approach with the Foldy-Wouthuysen (F-W) method. The F-W-expansion is in principle a formal expansion of the unbounded Dirac operator in c^{-2} which is used by physicists to compute relativistic corrections. (It became popular since the terms in (A.7) have a nice physical interpretation.) Since the perturbations become more and more singular it is quite remarkable that this expansion (interpreted appropriately) yields formally correct results (see e.g. [10, 12]).

Let $f(\lambda, c^{-2}, \omega, \omega')$ be the Dirac scattering amplitude

$$f(\lambda, c^{-2}, \omega, \omega') := -2\pi i\frac{1}{k^d}(S(\lambda)-1)(\omega,\omega'), \quad \text{a.e. } \lambda\in I, \quad \omega,\omega'\in S^2. \tag{A.1}$$

Then we get by (5.85) the following expansion:

$$\begin{aligned} f(\lambda, c^{-2}, \omega, \omega') &= f^{(0)}(\lambda, \omega, \omega') \\ &\quad + c^{-2}\Bigg[\frac{\lambda^2}{2m}\frac{df^{(0)}(\lambda,\omega,\omega')}{d\lambda} - \frac{\lambda}{4\pi}\int_{\mathbb{R}^3} d^3x \bar{\psi}^s_-(k^s\omega, x) v(x) \psi^s_+(k^s\omega', x) \\ &\quad - \frac{1}{8\pi m}\int_{\mathbb{R}^3} d^3x (\overline{\boldsymbol{\sigma}\mathbf{p}\psi^s_-}(k^s\omega))(x) v(x) (\boldsymbol{\sigma}\mathbf{p}\psi^s_+(k^s\omega'))(x)\Bigg] \\ &\quad + O(c^{-4}), \end{aligned} \tag{A.2}$$

where

$$\begin{aligned} f^{(0)}(\lambda,\omega,\omega') &= -2\pi i \frac{1}{k^s}(S^{(0)}(\lambda) - 1)(\omega,\omega') \\ &= -\frac{2m}{4\pi}\int_{\mathbb{R}^3} d^3x\, e^{-ik^s\omega x} v(x) \psi^s_+(k^s\omega', x). \end{aligned} \tag{A.3}$$

This expansion of the scattering amplitude $f(\lambda, c^{-2}, \omega, \omega')$ coincides with the expansion of the scattering amplitude $t(\lambda, c^{-2}, \omega, \omega')$ of [14] after multiplying $t(\lambda, c^{-2}, \omega, \omega')$ by a factor $-2\pi^2 \frac{k^d}{ck_0} = -2\pi^2 2m(1+\lambda(2mc^2)^{-1})$ and expanding the function $e(\lambda, c^{-2}) = \lambda(1+\lambda(2mc^2)^{-1})$ with respect to c^{-2}. (We do not average over spin states in order to keep greater generality.)

Next define the Pauli operators H_1^0, H_1 in $L^2(\mathbb{R}^3)^2$ (see e.g. [12, 34])

$$H_1^0 = -\frac{\Delta}{2m}, \qquad H_1 = -\frac{\Delta}{2m} + V, \qquad \mathscr{D}(H_1^0) = \mathscr{D}(H_1) = H^{2,2}(\mathbb{R}^3)^2, \tag{A.4}$$

where we assume that V is the maximal multiplication operator by the real-valued function $v(x)$ with $v \in C_0^\infty(\mathbb{R}^3)$ for simplicity. (Here we suppress the trivial spin dependence in H_1^0, H_1.) Then

$$\sigma_{\text{ess}}(H_1^0) = \sigma_{\text{ac}}(H_1^0) = [0, \infty). \tag{A.5}$$

The first order F-W operators in $L^2(\mathbb{R}^3)^2$ are now defined by (see e.g. [10, 12])

$$\begin{gathered} H^0_{\text{FW}}(c) := -\frac{\Delta}{2m} - \frac{1}{8c^2m^3}\Delta^2, \qquad H_{\text{FW}}(c) := H^0_{\text{FW}}(c) + W(c), \\ \mathscr{D}(H^0_{\text{Fw}})(c) = \mathscr{D}(H_{\text{FW}}(c)) = H^{2,4}(\mathbb{R}^3)^2, \end{gathered} \tag{A.6}$$

where

$$W(c) := V + \frac{1}{4m^2c^2}\Big[\frac{1}{2}\Delta V + \boldsymbol{\sigma}(\nabla V) \wedge \mathbf{p}\Big], \qquad \mathbf{p} = -i\nabla. \tag{A.7}$$

We have

$$\begin{gathered} \sigma_{\text{ess}}(H^0_{\text{FW}}(c)) = \sigma_{\text{ac}}(H^0_{\text{FW}}(c)) = \Big(-\infty, \frac{1}{2}mc^2\Big], \\ H^0_{\text{FW}}(c)\psi^0_{\text{FW}} = \lambda\psi^0_{\text{FW}}, \qquad \psi^0_{\text{FW}}(k^{\text{FW}}\omega, x) = e^{ik^{\text{FW}}\omega x}, \end{gathered} \tag{A.8}$$

where

$$k^{\text{FW}} := \left[2m^2c^2 - 2m^2c^2\left(1 - \frac{4\lambda}{2mc^2}\right)^{1/2}\right]^{1/2} = (2m\lambda)^{1/2}\left(1 + \frac{\lambda}{4mc^2}\right) + O(c^{-4}). \tag{A.9}$$

Before we compare the results of our approach and the F-W-method in connection with scattering theory, let us briefly recall the corresponding facts for eigenvalues. For simplicity assume E_0 to be a nondegenerate bound state of H_1, i.e., $H_1\psi_0 = E_0\psi_0$ for some $\psi_0 \in H^{2,2}(\mathbb{R}^3)^2$, $\|\psi_0\| = 1$. Then the first-order correction term E_1 to the corresponding eigenvalue of the Dirac operator $c\boldsymbol{\alpha}\mathbf{p} + (\beta - 1)mc^2 + V$ is given by $E_0 + \frac{1}{c^2}E_1$ with [10, 11],

$$E_1 = \frac{1}{4m^2}(\boldsymbol{\sigma}\mathbf{p}\psi_0, (V - E_0)\boldsymbol{\sigma}\mathbf{p}\psi_0). \tag{A.10}$$

In contrast to this simple formula the F-W method has some conceptual difficulties since for negative energies there exist no bound states. Nevertheless a formal perturbation calculation yields

$$E_1 = \frac{1}{4m^2}\left(\psi_0, \left[-\frac{\mathbf{p}^4}{2m} + \frac{1}{2}\Delta V + \boldsymbol{\sigma}(\nabla V) \wedge \mathbf{p}\right]\psi_0\right). \tag{A.11}$$

One can show that (A.10) and (A.11) are equal if e.g. $\partial_{x_j}\partial_{x_l}V \in C^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, $1 \leq j,\, l \leq 3$. The result can be explained in terms of spectral concentration as shown in [12]. However, we emphasize that expression (A.10) is simpler than the traditional F-W-formula (A.11) and at the same time it is based on an analytic expansion of the Dirac eigenvalue (rest energy subtracted) with respect to c^{-2} as opposed to the somewhat artificial spectral concentration approach. Moreover, (A.11) requires much more smoothness of the potential V than (A.10) and, in particular, excludes Coulomb-type singularities (which are included in [10, 11]).

Now we turn to scattering theory. Since we are interested in relativistic corrections to nonrelativistic scattering quantities for a fixed $\lambda > 0$, we consider $\lambda \in \left(0, \frac{1}{2}mc^2\right)$ and choose c large enough. According to our conventions the F-W scattering amplitude $f_{\mathrm{FW}}(\lambda, c^{-2}, \omega, \omega')$ for a.e. $\lambda \in \left(0, \frac{1}{2}mc^2\right)$ is defined by

$$\begin{aligned} f_{\mathrm{FW}}(\lambda, c^{-2}, \omega, \omega') :=& -\frac{1}{4\pi}g(\lambda, c^{-2}) \int_{\mathbb{R}^3} d^3x\, e^{-ik^{\mathrm{FW}}\omega x} \\ &\times W(c)[1 - (H_{\mathrm{FW}} - \lambda - i0)^{-1}W(c)]\, e^{ik^{\mathrm{FW}}\omega'(\cdot)}, \\ &\omega, \omega' \in S^2, \\ g(\lambda, c^{-2}) :=& \frac{k^d}{ck_0}(1 + k_0^2) = 2m\left(1 + \frac{\lambda}{mc^2}\right) + O(c^{-4}). \end{aligned} \tag{A.12}$$

Expanding (A.12) in powers of c^{-2} gives

$$f_{\mathrm{FW}}(\lambda, c^{-2}, \omega, \omega') = f_{\mathrm{FW}}^{(0)}(\lambda, \omega, \omega') + c^{-2}f_{\mathrm{FW}}^{(1)}(\lambda, \omega, \omega') + O(c^{-4}), \tag{A.13}$$

where

$$\begin{aligned} f_{\mathrm{FW}}^{(0)}(\lambda, \omega, \omega') &= -\frac{2m}{4\pi}\int_{\mathbb{R}^3} d^3x\, e^{-ik^s\omega x}(V[1 - (H_1 - \lambda - i0)^{-1}V]\, e^{ik^s\omega'(\cdot)})(x) \\ &= -\frac{2m}{4\pi}\int_{\mathbb{R}^3} d^3x\, e^{-ik^s\omega x}v(x)\psi_+^s(k^s\omega', x) = f^{(0)}(\lambda, \omega, \omega') \end{aligned} \tag{A.14}$$

by (A.3) and

$$f_{\mathrm{FW}}^{(1)}(\lambda, \omega, \omega') = \frac{\lambda^2}{2m}\frac{df^{(0)}(\lambda, \omega, \omega')}{d\lambda} - \frac{2m}{4\pi}\int_{\mathbb{R}^3} d^3x\, e^{-ik^s\omega x}(K(\lambda)\, e^{ik^s\omega'(\cdot)})(x) \tag{A.15}$$

with

$$K(\lambda) := \frac{1}{4m^2}\left[\tfrac{1}{2}\Delta V + \boldsymbol{\sigma}(\nabla V)\wedge\mathbf{p}\right](1-R_1V)$$
$$-\frac{1}{4m^2}VR_1\left[\tfrac{1}{2}\Delta V + \boldsymbol{\sigma}(\nabla V)\wedge\mathbf{p}\right]$$
$$+VR_1\left\{-\frac{\Delta^2}{8m^3}+\frac{1}{4m^2}\left[\tfrac{1}{2}\Delta V + \boldsymbol{\sigma}(\nabla V)\wedge\mathbf{p}\right]\right\}R_1V$$
$$+\frac{\lambda}{m}V(1-R_1V)+\frac{\lambda^2}{2m}VR_1^2V$$
$$=\frac{1}{4m^2}(1-VR_1)\left[\tfrac{1}{2}\Delta V + \boldsymbol{\sigma}(\nabla V)\wedge\mathbf{p}\right](1-R_1V)-\frac{1}{8m^3}VR_1(\boldsymbol{\sigma}\mathbf{p})^4R_1V$$
$$+\frac{\lambda}{m}V(1-R_1V)+\frac{\lambda^2}{2m}VR_1^2V,$$
$$R_1 := (H_1-\lambda-i0)^{-1}, \quad \psi_{\pm}^s(k^s\omega,x)=((1-(H_1-\lambda\pm i0)^{-1}V)e^{ik^s\omega(\cdot)})(x). \tag{A.16}$$

We note that

$$[\boldsymbol{\sigma}\mathbf{p},V]\boldsymbol{\sigma}\mathbf{p}=\boldsymbol{\sigma}\mathbf{p}V\boldsymbol{\sigma}\mathbf{p}-V(\boldsymbol{\sigma}\mathbf{p})^2,$$
$$\int_{\mathbb{R}^3} d^3x\bar{\psi}_-^s(k^s\omega,x)\left(\left[\tfrac{1}{2}\Delta V + \boldsymbol{\sigma}(\nabla V)\wedge\mathbf{p}\right]\psi_+^s(k^s\omega)\right)(x)$$
$$=\int_{\mathbb{R}^3} d^3x\bar{\psi}_-^s(k^s\omega,x)([\boldsymbol{\sigma}\mathbf{p},V]\boldsymbol{\sigma}\mathbf{p}\psi_+^s(k^s\omega))(x) \tag{A.17}$$

since

$$\int_{\mathbb{R}^3} d^3x\bar{\psi}_-^s(k^s\omega,x)([\Delta,V]\psi_+^s(k^s\omega))(x)=0. \tag{A.18}$$

Using (A.17) and (A.8) we finally obtain

$$\int_{\mathbb{R}^3} d^3x\,e^{-ik^s\omega x}(K(\lambda)e^{ik^s\omega'(\cdot)})(x)$$
$$=\int_{\mathbb{R}^3} d^3x\,e^{-ik^s\omega x}\left\{\left(\frac{1}{4m^2}(1-VR_1)\left[\tfrac{1}{2}\Delta V + \boldsymbol{\sigma}(\nabla V)\wedge\mathbf{p}\right](1-R_1V)\right.\right.$$
$$\left.\left.-\frac{1}{8m^3}VR_1(\boldsymbol{\sigma}\mathbf{p})^4R_1V+\frac{\lambda}{m}V(1-R_1V)+\frac{\lambda^2}{2m}VR_1^2V\right)e^{ik^s\omega'(\cdot)}\right\}(x)$$
$$=\int_{\mathbb{R}^3} d^3x\,e^{-ik^s\omega x}\left\{\left(\frac{1}{4m^2}(1-VR_1)[\boldsymbol{\sigma}\mathbf{p},V]\boldsymbol{\sigma}\mathbf{p}(1-R_1V)\right.\right.$$
$$\left.\left.-\frac{1}{8m^3}VR_1(\boldsymbol{\sigma}\mathbf{p})^4R_1V+\frac{\lambda}{m}V(1-R_1V)+\frac{\lambda^2}{2m}VR_1^2V\right)e^{ik^s\omega'(\cdot)}\right\}(x)$$
$$=\frac{\lambda}{2m}\int_{\mathbb{R}^3} d^3x\,e^{-ik^s\omega x}\{((1-VR_1)V(1-R_1V))e^{ik^s\omega'(\cdot)}\}(x)$$
$$+\frac{1}{4m^2}\int_{\mathbb{R}^3} d^3x\,e^{-ik^s\omega x}\{((1-VR_1)(\boldsymbol{\sigma}\mathbf{p}V\boldsymbol{\sigma}\mathbf{p})(1-R_1V))e^{ik^s\omega'(\cdot)}\}(x), \tag{A.19}$$

and hence (A.15) coincides with (A.2). However, in analogy to the bound state case mentioned before, (A.2) is much simpler than (A.15) and requires less smoothness properties of V. [In order to speed up our treatment we did not factor V into $v^{1/2}|v|^{1/2}$ and symmetrize the expressions in (A.12)–(A.19). This can be done as in Sect. 5 and we omit the details.]

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